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A primer on rotational collective enhancements in even-even nuclei

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A primer on rotational collective enhancements in even-even nuclei

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The enhancement of the level density for deformed nuclei relative to the level density in spherical nuclei is calculated. The qualitative behavior of the enhancement factor as a function of excitation energy is explained, and a prescription for a more quantitative description of this behavior is suggested. The results presented here can be found elsewhere in the literature, however the treatments of this topic are dispersed in the literature, are often terse, and require some familiarity with disparate branches of physics. The emphasis of this paper is on step-by-step derivations of the physics and mathematics used in the calculation of level densities and rotational enhancement factors. Pertinent techniques from thermodynamics and group theory are introduced. Appendices provide detailed introductions to the principal mathematical tools.

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I. INTRODUCTION

Early on in the history of statistical level-density calculations, it was understood [1] that level-counting in a deformed nucleus needed to include the rotational levels, in addition to the intrinsic states normally counted in a spherical system. However, the implications of this fact were not truly appreciated until the seminal paper by Bjørnholm *et al.* [2] was published. In [2], the authors explain the origin of the enhancement in level density for deformed nuclei, compared to spherical systems, and derive enhancement factors for different nuclear shapes. These enhancement factors have been widely used in the subsequent literature and, for example, have played a critical role in the interpretation of fission data [3, 4]. Since 1974, surprisingly little work has been done on the topic of collective enhancement factors in rotational nuclei, and except for a few isolated publications (e.g., [5]), even less has been said about how the collective enhancement factors behave as a function of excitation energy.

The paper by Bjørnholm *et al.* forms the basis of most subsequent discussions of collective enhancement factors in the literature. The article itself is difficult to follow for the non-expert, because it assumes knowledge of disparate branches of physics. Much of the background required to follow the derivation in [2] is dispersed in the literature and, sometimes, poorly explained. In this paper we present and overview of the physics and mathematics underlying the results in [2], with a special emphasis on giving detailed, step-by-step derivations.

In broad terms, this paper covers the calculation of level densities from single-particle states using techniques borrowed from thermodynamics in section II. Section III introduces tools from group theory to count levels in deformed nuclei with well-defined intrinsic symmetries. In section IV the behavior of collective enhancement factors as a function of excitation energy is investigated using statistical techniques. Mathematical techniques that are especially important to the topics in this paper, or of more general pedagogic value, have been included in the appendices.

This paper can serve as a starting point for the topics covered herein, but the discussions are by no means comprehensive. For a more formal introduction, the reader is directed to the references quoted throughout the paper.

II. INTRINSIC LEVEL DENSITIES

This section introduces the basic concepts used to calculate nuclear level densities using methods of statistical mechanics. The distinction is made between state and level densities, and the role of angular momentum is described. A commonly-used level-counting technique based on the partition function of the system is introduced to obtain a formal expression for the state density in a spherical nucleus. As a practical example, the partition-function method is applied to the case of equally-spaced single-particle levels. We conclude with a brief discussion of more general applications of the partition-function method.

A. Bethe's formula for the angular-momentum distribution

In a 1937 paper [6], Hans Bethe described a procedure whereby the distribution of levels in a nucleus as a function of angular momentum could be deduced from a simple nuclear model. In this model, the nucleus is composed of n independent nucleons, each carrying the same spin j. The individual spins j couple to give the nucleus its total angular momentum J, with projection M on some arbitrary z axis. The nucleon spins j also have projections m_i on the z axis (where the index $i = 1, \dots, n$ designates each individual nucleon), and the total projection is

$$M = \sum_{i=1}^{n} m_i \tag{1}$$

In Bethe's model, the individual nucleon spins j have random, independent orientations in space. Therefore each projection m_i is sampled from an independent discrete uniform distribution. In other words, m_i can take on any value from $-j$ to j with equal probability (namely, $1/(2j+1)$), independently of the values taken by the other $m_{k \neq i}$ random variables. The problem tackled by Bethe was to determine the probability distribution of the total projection M within this simple model.

It can be shown that, for a sufficiently large number n of nucleons, M is approximately Gaussian-distributed. In [6] Bethe gives a concise argument for this, which does not constitute a rigorous proof. A robust proof that M follows a Gaussian distribution is provided by the powerful central limit theorem [7], which in its usual form states that if $X_1, X_2, \ldots, X_n$ are independent and identically-distributed random variables, each with mean μ and variance σ^2, then the random variable

$$\frac{X_1 + \cdots + X_n - n\mu}{\sqrt{n}\sigma} \tag{2}$$

has a distribution that tends to a Gaussian with mean 0 and variance 1 as $n \to \infty$. The power of the central-limit theorem resides in the fact that it holds for any probability distribution of the X_i. In the problem at hand, the random variables are the z projections m_i, each following a discrete uniform distribution over $[-j, j]$ with mean $\mu_i = 0$ and variance

$$\begin{aligned} \sigma_i^2 = \langle (m - \langle m \rangle)^2 \rangle = \langle m^2 \rangle &= \sum_{m_i=-j}^{j} m_i^2 \times \frac{1}{2j+1} \\ &= \frac{1}{3} j(j+1). \end{aligned} \tag{3}$$

Using the central-limit theorem, this means that for large-enough n, the quantity in Eq. (2),

$$\frac{1}{\sqrt{n}\sigma_i} \sum_{i=1}^{n} m_i = \frac{1}{\sqrt{n}\sigma_i} M, \tag{4}$$

tends to a Gaussian distribution with mean 0 and variance 1, which we denote by $f_G(x; 0, 1)$. It follows that the probability distribution for the total projection M is [45]

$$\begin{aligned} p_n(M) &= \frac{1}{\sqrt{n}\sigma_i} \times f_G\left(\frac{M}{\sqrt{n}\sigma_i}; 0, 1\right) \\ &= \frac{1}{\sqrt{n}\sigma_i} \times \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{M}{\sqrt{n}\sigma_i}\right)^2\right] \\ &= \left[\frac{2\pi}{3} n j(j+1)\right]^{-1/2} \exp\left[-\frac{3M^2}{2nj(j+1)}\right], \end{aligned} \tag{5}$$

where Eq. (3) has been used in the last step. This is precisely the form derived by Bethe in Eq. (34) of reference [6].

In order to take advantage of Eq. (5) and extract a level density $\rho(E, J)$ as a function of excitation energy E and angular momentum J, we introduce the concept of a state density, denoted by $w(E, J)$. Unlike the level density, the state density takes into account the $2J + 1$, z-projection degeneracy of each level with spin J. Mathematically, the level and state densities are related by

$$w(E, J) = (2J + 1)\rho(E, J). \tag{6}$$

And the corresponding total densities are

$$\rho(E) \equiv \sum_J \rho(E, J) \tag{7a}$$

$$w(E) \equiv \sum_J w(E, J) = \sum_J (2J + 1)\rho(E, J). \tag{7b}$$

The density of states with a given projection M is

$$w(E, M) = w(E) \times p_n(M), \tag{8}$$

where $p_n(M)$ is the Gaussian distribution in Eq. (5), and $w(E)$ is the total state density given by Eq. (7b). For the sake of generality, we keep the Gaussian distribution in its general form, with $\sigma \equiv \sqrt{n}\sigma_i$, with σ_i given by Eq. (3). Then

$$w(E,M) = w(E) \times \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{M^2}{2\sigma^2}\right]. \tag{9}$$

Now, the states with projection $M = J$ are those with spin $J, J+1, \ldots$, while the states with projection $M = J+1$ are those with spin $J+1, J+2, \ldots$. Therefore, the density of levels with a given spin J is obtained by taking the difference of state densities

$$\begin{aligned} \rho(E,J) &= w(E, M=J) - w(E, M=J+1) \\ &\approx -w(E) \times \left.\frac{dp_n(M)}{dM}\right|_{M=J+1/2} \\ &= w(E) \times \frac{2J+1}{2\sqrt{2\pi}\sigma^3} \exp\left[-\frac{(J+1/2)^2}{2\sigma^2}\right], \end{aligned} \tag{10}$$

where the approximation in the second step works best for large values of J. The quantity σ^2 in this context is often referred to as the "spin cutoff", because it determines how much the larger values of J are inhibited in Eq. (10).

B. Level density for a spherical nucleus

Equation (10) tells us that in order to calculate the level density, we must obtain the total state density. This is not a simple task, and although direct counting techniques have been used in certain cases, they are not feasible when the number of levels is very large. We will focus our discussion on statistical methods that estimate the number of states produced by distributing nucleons in a set of single-particle levels. These methods are more amenable to problems where very large numbers of states are generated.

1. *Partition-function method*

We begin with the simple case of a toy nucleus with only one type of nucleon (i.e., proton or neutron, but not both), and where only the energy is a constant (e.g., the number of nucleons need not be conserved). We assume that the exclusion principle is enforced (i.e., we define each single-particle level such that it can hold 0 or 1 particle), in this manner, the counting of many-body states formed by different configurations of nucleons in the single-particle levels produce a state density, with proper accounting of the z-projection degeneracy (for example, a spin-7/2 state is described as 8 degenerate states, each of which can hold at most 1 particle). This is of course an unrealistic example, but will serve to illustrate the statistical approach in the simplest way.

If we could somehow calculate the energy E_i of each many-body state produced by an arrangement of the individual particles in single-particle levels, then the state density could be written as a sum of Dirac-delta functions

$$w(E) = \sum_i \delta\left(E - E_i\right). \tag{11}$$

Equation (11) is technically correct for the simple nuclear model we wish to describe, but cumbersome to work with. Because of the delta functions involved in the sum, it is difficult to see how the sum could be simplified, even if we had an explicit expression for the state energies E_i. For the sake of mathematical tractability, we choose to work instead with the Laplace transform of Eq. (11),

$$Z(\beta) \equiv \mathcal{L}[w(E)] = \int_0^\infty w(E) e^{-\beta E} dE. \tag{12}$$

We denote this Laplace transform by the symbol $Z(\beta)$ with malice aforethought, because Eq. (12) is also the definition of a thermodynamic partition function. Thus we have made a connection between the state density of nuclear configurations and the formalism of statistical mechanics.

If the partition function $Z(\beta)$ could be calculated by independent means then, in principle, Eq. (12) could be inverted to produce the state density $w(E)$. We assume that such an expression for the partition function has been found and look for a formal solution. The state density is the inverse Laplace transform of Eq. (12) [8] [46]

$$w(E) = \mathcal{L}^{-1}[Z(\beta)] = \frac{1}{2\pi i}\int_{-i\infty}^{+i\infty} Z(\beta)e^{\beta E}d\beta. \tag{13}$$

In order to dispel the appearance that we have engaged in circular reasoning by writing down Eqs. (12) and (13), we emphasize the point that we are in fact shifting our tactics to calculating the partition function $Z(\beta)$ first, rather than attempting to tackle the density of states $w(E)$ directly. To this end, we note that the integral in Eq. (13) can be estimated using the saddle-point approximation, also know as the method of steepest descents, or the stationary-phase approximation. The saddle-point approximation is described in appendix A, but it amounts to the statement that the integral in Eq. (13) is dominated by the "behavior" of the integrand at a single, special point in the complex plane: a saddle point. The saddle point, for a given energy E, is determined by the condition

$$\left.\frac{\partial}{\partial\beta}\ln Z(\beta)\right|_{\beta=\beta_0} + E = 0, \tag{14}$$

where β_0 denotes the saddle-point position. The saddle-point approximation then yields

$$w(E) \approx \left.\frac{e^{\ln Z(\beta)+\beta E}}{\sqrt{2\pi}\left[\frac{\partial^2}{\partial\beta^2}\ln Z(\beta)\right]^{1/2}}\right|_{\beta=\beta_0}, \tag{15}$$

where β_0 has been determined by solving Eq. (14). Note that we have resisted the temptation to simplify the exponential in Eq. (15). This was done deliberately to isolate the quantity

$$S(\beta) \equiv \ln Z(\beta) + \beta E, \tag{16}$$

which is recognizable as the entropy of the system at fixed energy [9]. In fact, the parameter β in Eq. (16) plays the role of a Lagrange multiplier, constraining the average energy of the system.

Suppose we now want to describe a gas composed of A nucleons with total energy E. This is the situation encountered in the grand canonical ensemble in statistical mechanics. The expression for the state density, Eq. (11), must be modified somewhat to read

$$w(A,E) = \sum_{n,i}\delta\left(A-n\right)\delta\left(E-E_i(n)\right), \tag{17}$$

where $E_i(n)$ is now the energy of the ith quantum state, consisting of n nucleons. In order to better understand Eq. (17), it is useful to make the connection with individual nucleons filling single-particle orbitals. Thus, if the index ν is chosen to label single-particle state (as opposed to the index i in Eq. (17), which labels many-body states of the system), $n_\nu = 0$, or 1 particle can be placed in level ν of energy ϵ_ν, subject to the constraints

$$\begin{aligned}\sum_\nu n_\nu &= n \\ \sum_\nu n_\nu\epsilon_\nu &= E_i(n).\end{aligned} \tag{18}$$

Thus a given arrangement $\{n_1, n_2, \dots\}$ of n particles among the single-particle levels $\{\epsilon_1, \epsilon_2, \dots\}$ produces a many-body state of energy $E_i(n)$, according to Eq. (18) [47]. Among all possible many-body states formed in this way, Eq. (17) counts only those corresponding to configurations of $n = A$ particles and energy $E_i(n) = E$. The partition function (usually called the grand partition function in this case) is written [10]

$$Z(\alpha,\beta) \equiv \int_0^\infty \int_0^\infty w(A,E)e^{\alpha A-\beta E} dA\, dE. \tag{19}$$

The inverse Laplace transform gives the density of states

$$w(E) = \left(\frac{1}{2\pi i}\right)^2 \int_{-i\infty}^{+i\infty} \int_{-i\infty}^{+i\infty} Z(\alpha,\beta)e^{-\alpha A+\beta E} d\alpha\, d\beta. \tag{20}$$

The saddle-point approximation can be applied in this case and produces two simultaneous equations defining the location (α_0, β_0) of the saddle

$$\frac{\partial}{\partial\beta} \ln Z(\alpha,\beta)\bigg|_{\alpha=\alpha_0,\beta=\beta_0} + E = 0 \tag{21a}$$

$$\frac{\partial}{\partial\alpha} \ln Z(\alpha,\beta)\bigg|_{\alpha=\alpha_0,\beta=\beta_0} - A = 0, \tag{21b}$$

and the state density itself is given by the generalization of Eq. (15)

$$w(A,E) \approx \frac{e^{\ln Z(\alpha,\beta)-\alpha A+\beta E}}{2\pi\sqrt{D}}\bigg|_{\alpha=\alpha_0,\beta=\beta_0}, \tag{22}$$

where D is the determinant of a 2×2 matrix of second-order partials

$$D = \det \begin{vmatrix} \frac{\partial^2}{\partial\alpha^2} \ln Z(\alpha,\beta) & \frac{\partial^2}{\partial\alpha\partial\beta} \ln Z(\alpha,\beta) \\ \frac{\partial^2}{\partial\beta\partial\alpha} \ln Z(\alpha,\beta) & \frac{\partial^2}{\partial\beta^2} \ln Z(\alpha,\beta) \end{vmatrix} \tag{23}$$

It's not hard to see how this process can be generalized to include more constants of motion. For example, we could impose individual constraints on the number N of neutrons and Z of protons, or we could count only those configurations of nucleons with a specific spin $J_i(n)$ and parity $\pi_i(n)$. In general if there are m constants of motion X_j (where $j = 1, 2, \ldots, m$) in addition to the energy of the system, the state density is given by the inverse Laplace transform

$$w(X_1,\ldots,X_m,E) = \left(\frac{1}{2\pi i}\right)^{m+1} \underbrace{\int_{-i\infty}^{+i\infty} \cdots \int_{-i\infty}^{+i\infty}}_{\times m+1} Z(\alpha_1,\ldots,\alpha_m,\beta)e^{\beta E-\sum_{j=1}^m \alpha_j X_j} \, d\alpha_1 \ldots d\alpha_m\, d\beta. \tag{24}$$

The saddle-point approximation can be applied to this multi-dimensional integral and yields

$$w(X_1,\ldots,X_m,E) \approx \frac{e^{\ln Z(\alpha_1,\ldots,\alpha_m,\beta)+\beta E-\sum_{j=1}^m \alpha_j X_j}}{(2\pi)^{(m+1)/2}\sqrt{D}}\bigg|_{\alpha_j=\alpha_j^{(0)},\beta=\beta_0}, \tag{25}$$

where the expression is evaluated at the saddle-point location $(\alpha_1^{(0)}, \cdots, \alpha_m^{(0)}, \beta_0)$ obtained by solving the set of $m+1$ simultaneous equations for the Lagrange multipliers $\alpha_1, \ldots, \alpha_m, \beta$

$$\begin{cases} \frac{\partial}{\partial\beta} \ln Z(\alpha_1,\ldots,\alpha_m,\beta)\Big|_{\alpha_j=\alpha_j^{(0)},\beta=\beta_0} + E = 0 \\ \frac{\partial}{\partial\alpha_k} \ln Z(\alpha_1,\ldots,\alpha_m,\beta)\Big|_{\alpha_j=\alpha_j^{(0)},\beta=\beta_0} - X_k = 0 \qquad k = 1,\ldots,m. \end{cases} \tag{26}$$

The quantity D in Eq. (25) is the determinant of an $(m+1) \times (m+1)$ matrix with elements

$$D_{ij} = \begin{cases} \frac{\partial^2}{\partial \alpha_i \partial \alpha_j} \ln Z(\alpha_1, \ldots, \alpha_m, \beta) & 1 \leq i, j \leq m \\ \frac{\partial^2}{\partial \alpha_i \partial \beta} \ln Z(\alpha_1, \ldots, \alpha_m, \beta) & i \neq m+1, j = m+1 \\ \frac{\partial^2}{\partial \beta \partial \alpha_j} \ln Z(\alpha_1, \ldots, \alpha_m, \beta) & i = m+1, j \neq m+1 \\ \frac{\partial^2}{\partial \beta^2} \ln Z(\alpha_1, \ldots, \alpha_m, \beta) & i = m+1, j = m+1 \end{cases} \tag{27}$$

2. *The partition function for non-interacting fermions*

In the previous section we equated the problem of calculating the state density to that of calculating the partition function for the system, and we obtained a formal inversion formula to calculate the state density from the partition function. The partition function consists of a sum over all possible configurations of the system with a given energy, number of particles, etc. This aspect of the partition function sets the stage for further simplifications.

We return to the case of the grand partition function defined in Eq. (19) for a system of A particles with total energy E. We insert the explicit state density given in Eq. (17) into the definition of the partition function in Eq. (19) [11]

$$\begin{aligned} Z(\alpha, \beta) &= \int_0^\infty \int_0^\infty w(A, E) e^{\alpha A - \beta E} dA\, dE \\ &= \sum_{n,i} e^{\alpha n - \beta E_i(n)}. \end{aligned} \tag{28}$$

The sum in Eq. (28) extends over all possible numbers n of nucleons, distributed in all possible ways among the single-particle states, where each such configuration is labeled by the index i. This sum includes the case of interest with A particles in the configuration(s) giving the system a total energy E. Unfortunately, the quantity of interest, which appears in Eqs. (21) and (22), is the logarithm of the partition function, and not the partition function itself. The logarithm of the sum in Eq. (28) is not a particularly tractable form to work with.

In order to reduce Eq. (28) further, we us Eq. (18) to express the number of particles n and energies $E_i(n)$ in terms of the occupation numbers n_ν of the single-particle states,

$$\begin{aligned} \sum_{n,i} e^{\alpha n - \beta E_i(n)} &= \sum_{n,i} e^{\alpha \sum_\nu n_\nu - \beta \sum_\nu n_\nu \epsilon_\nu} \\ &= \sum_{n,i} e^{\sum_\nu n_\nu (\alpha - \beta \epsilon_\nu)} \\ &= \sum_{n,i} \left[\prod_\nu e^{n_\nu (\alpha - \beta \epsilon_\nu)} \right]. \end{aligned} \tag{29}$$

It is important to remember that, in Eq. (29), each set of indices n, i defines a particular set of values for the occupation numbers $n_1, n_2, \ldots$, and that the sum covers all possible such configurations. Let s be the number of single-particle levels (i.e., $\nu = 1, \ldots, s$). Then each of the s terms in the square brackets in Eq. (29) can have one of two values, depending on whether $n_\nu = 0$ or 1 (the Pauli exclusion principle does not allow any other values for n_ν). All the terms in the sum over n, i are obtained by considering all possible binary numbers $n_1 n_2 \ldots n_s$, each of which defines a unique value of the product in the square brackets. There are 2^s such binary numbers. The same complete set of products can be spanned by letting the factors $\nu = 2, \ldots, s$ take on all possible values for each of the two possible values of the first ($\nu = 1$) factor, that is

$$\begin{aligned} \sum_{n,i} \left[\prod_{\nu=1}^{s} e^{n_\nu (\alpha - \beta \epsilon_\nu)} \right] &= e^{n_1 (\alpha - \beta \epsilon_1)} \Big|_{n_1 = 0} \times \sum_{n',i'} \left[\prod_{\nu=2}^{s} e^{n_\nu (\alpha - \beta \epsilon_\nu)} \right] \\ &\quad + e^{n_1 (\alpha - \beta \epsilon_1)} \Big|_{n_1 = 1} \times \sum_{n',i'} \left[\prod_{\nu=2}^{s} e^{n_\nu (\alpha - \beta \epsilon_\nu)} \right] \\ &= \left[1 + e^{\alpha - \beta \epsilon_1} \right] \times \sum_{n',i'} \left[\prod_{\nu=2}^{s} e^{n_\nu (\alpha - \beta \epsilon_\nu)} \right], \end{aligned} \tag{30}$$

where the indices n', i' have been primed to indicate that they apply to the reduced set of single-particle levels $\nu = 2, \ldots, s$. This line of reasoning can be applied recursively to Eq. (30), and the sum over n, i is transformed into a product over ν,

$$\begin{aligned} \sum_{n,i} \left[\prod_{\nu=1}^{s} e^{n_\nu(\alpha - \beta\epsilon_\nu)} \right] &= \left[1 + e^{\alpha - \beta\epsilon_1}\right] \times \cdots \times \left[1 + e^{\alpha - \beta\epsilon_s}\right] \\ &= \prod_{\nu=1}^{s} \left[1 + e^{\alpha - \beta\epsilon_\nu}\right], \end{aligned} \tag{31}$$

and therefore,

$$\ln Z(\alpha, \beta) = \sum_{\nu=1}^{s} \ln\left(1 + e^{\alpha - \beta\epsilon_\nu}\right). \tag{32}$$

Eq. (32) is a simplified form of the logarithm of the partition function given by Eq. (28).

3. Continuum limit

A further, useful approximation to Eq. (32) is obtained by going to the continuum limit and replacing the sum with an integral. If we denote the density of single-particle levels by $g(\epsilon)$, where

$$g(\epsilon) = \sum_{\nu=1}^{s} \delta(\epsilon - \epsilon_\nu), \tag{33}$$

then we can write the exact result

$$\ln Z(\alpha, \beta) = \int_0^\infty g(\epsilon) \ln\left(1 + e^{\alpha - \beta\epsilon}\right) d\epsilon \tag{34}$$

In the next section, we will approximate the density in Eq. (33) by a constant function of energy (i.e., $g(\epsilon) \equiv g_0$). In that case, the integral in Eq. (34) cannot be reduced to a closed form for arbitrary values of α. However, in the special case $\alpha = 0$, we have the result for any $\beta > 0$ [12]

$$\int_0^\infty \ln\left(1 + e^{-\beta\epsilon}\right) d\epsilon = \frac{\pi^2}{12\beta} \tag{35}$$

4. The equidistant-level model

To obtain a concrete expression from Eq. (34), we must make some assumptions about the distribution of the single-particle states. The simplest non-trivial model assumes that the single-particle states are equidistant (i.e., that $\epsilon_\nu = (\nu - 1)\Delta\epsilon$ for $\nu = 1, 2, \cdots$, where $\Delta\epsilon$ is a constant). We approximate this by taking $g(\epsilon) \equiv g_0$ in Eq. (34). Note that we've implicitly assumed that there are infinitely-many single-particle levels (i.e., we've assumed that $s \to \infty$ in Eq. (32)). This assumption will make it possible to evaluate the integral in Eq. (34) in closed form, using Eq. (35).

We mentioned in the previous section that the integral in Eq. (34) could not be evaluated explicitly for arbitrary values of α. We assume that $\alpha > 0$ and $\beta > 0$ in what follows. Since we cannot obtain a closed form for the integral, we can think of expanding the logarithm in an infinite series instead using [12]

$$\ln(1 + x) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{x^k}{k} \qquad -1 < x \leq 1. \tag{36}$$

Note the constraint on x in this expansion. The restriction on the values of x poses a problem when we try to evaluate the integral in Eq. (34)

$$\ln Z(\alpha,\beta) = g_0 \int_0^\infty \ln\left(1+e^{\alpha-\beta\epsilon}\right) d\epsilon, \tag{37}$$

because $e^{\alpha-\beta\epsilon} \leq 1$ when $\epsilon \geq \alpha/\beta$, but $e^{\alpha-\beta\epsilon} > 1$ when $\epsilon < \alpha/\beta$ (remember we've assumed α and β are both strictly positive). Therefore it seems useful to break up the integral in Eq. (37) into two contributions

$$\begin{aligned} \ln Z(\alpha,\beta) &= g_0 \int_0^\infty \ln\left(1+e^{\alpha-\beta\epsilon}\right) d\epsilon \\ &= g_0 \int_0^{\alpha/\beta} \ln\left(1+e^{\alpha-\beta\epsilon}\right) d\epsilon + g_0 \int_{\alpha/\beta}^\infty \ln\left(1+e^{\alpha-\beta\epsilon}\right) d\epsilon. \end{aligned} \tag{38}$$

The second integral can be cast into the form in Eq. (35) by the variable substitution $x \equiv \epsilon - \alpha/\beta$, then

$$\ln Z(\alpha,\beta) = g_0 \int_0^{\alpha/\beta} \ln\left(1+e^{\alpha-\beta\epsilon}\right) d\epsilon + \underbrace{g_0 \int_0^\infty \ln\left(1+e^{-\beta x}\right) dx}_{\frac{\pi^2}{12\beta}}. \tag{39}$$

The first integral in Eq. (38) cannot be evaluated explicitly and requires a bit more work. We would like to use the expansion given by Eq. (36), but since the integration region is $0 \leq x \leq \alpha/\beta$, the exponential term is greater than 1. Therefore, we perform a bit of algebra to further break up the first integral in Eq. (39),

$$\begin{aligned} \ln Z(\alpha,\beta) &= g_0 \int_0^{\alpha/\beta} \ln\left[e^{\alpha-\beta\epsilon}\left(1+e^{-\alpha+\beta\epsilon}\right)\right] d\epsilon + \frac{g_0\pi^2}{12\beta} \\ &= g_0 \int_0^{\alpha/\beta} (\alpha-\beta\epsilon)\, d\epsilon + g_0 \int_0^{\alpha/\beta} \ln\left(1+e^{-\alpha+\beta\epsilon}\right) d\epsilon + \frac{g_0\pi^2}{12\beta}, \end{aligned} \tag{40}$$

where the exponential in the second integral of Eq. (40) is now less than 1 and the logarithm can therefore be expanded. For this integral we write

$$\begin{aligned} g_0 \int_0^{\alpha/\beta} \ln\left(1+e^{-\alpha+\beta\epsilon}\right) d\epsilon &= g_0 \int_0^{\alpha/\beta} d\epsilon \sum_{k=1}^\infty (-1)^{k+1} \frac{\left(e^{-\alpha+\beta\epsilon}\right)^k}{k} \\ &= g_0 \sum_{k=1}^\infty \frac{(-1)^{k+1}}{k} e^{-\alpha k} \int_0^{\alpha/\beta} d\epsilon\, e^{\beta k\epsilon} \\ &= \frac{g_0}{\beta} \sum_{k=1}^\infty \frac{(-1)^{k+1}}{k^2} - \frac{g_0}{\beta} \sum_{k=1}^\infty \frac{(-1)^{k+1}}{k^2} e^{-\alpha k}. \end{aligned} \tag{41}$$

The infinite series in the first term of Eq. (41) converges to $\pi^2/12$. This result can be derived by inserting the expansion of Eq. (36) into Eq. (35) for the case $\beta = 1$. The second term in Eq. (41) cannot be simplified in the same way, but it is typically neglected because of the $e^{-\alpha k}$ factors, which are small for sufficiently-large values of α. We can now return to Eq. (40)

$$\ln Z(\alpha,\beta) \approx g_0 \int_0^{\alpha/\beta} (\alpha-\beta\epsilon)\, d\epsilon + \frac{g_0\pi^2}{12\beta} + \frac{g_0\pi^2}{12\beta} = g_0 \int_0^{\alpha/\beta} (\alpha-\beta\epsilon)\, d\epsilon + \frac{g_0\pi^2}{6\beta}. \tag{42}$$

The remaining integral in Eq.(42) can be evaluated trivially, but we have refrained from doing so in order to introduce some physical quantities into the calculation. Namely, we can define the Fermi energy ϵ_F by filling the lowest single-particle levels to produce the ground-state energy E_0, and the total number of particles A according to

$$\int_0^{\epsilon_F} d\epsilon\, g_0 \equiv A \tag{43a}$$

$$\int_0^{\epsilon_F} d\epsilon\, g_0\epsilon \equiv E_0. \tag{43b}$$

Then we can write

$$\begin{aligned}\ln Z(\alpha,\beta) &\approx g_0\int_0^{\epsilon_F}(\alpha-\beta\epsilon)\,d\epsilon + g_0\int_{\epsilon_F}^{\alpha/\beta}(\alpha-\beta\epsilon)\,d\epsilon + \frac{g_0\pi^2}{6\beta}\\ &= \alpha A - \beta E_0 + \frac{g_0(\alpha-\beta\epsilon_F)^2}{2\beta} + \frac{g_0\pi^2}{6\beta}.\end{aligned} \tag{44}$$

The requisite partial derivatives for the saddle-point condition (Eq. (21)) can be obtained either from Eq. (34) or Eq. (44), both yield the same answer for $\alpha \gg 1$ (remember that we neglected the second sum in Eq. (41)). The first-order partials are

$$\frac{\partial}{\partial\alpha}\ln Z(\alpha,\beta) \approx g_0\frac{\alpha}{\beta} \tag{45a}$$

$$\frac{\partial}{\partial\beta}\ln Z(\alpha,\beta) \approx -E_0 - \frac{\pi^2 g_0}{6\beta^2} - \frac{g_0}{2\beta^2}(\alpha^2-\beta^2\epsilon_F). \tag{45b}$$

Combining Eqs. (21b), (43a) and (45a) we get the saddle-point condition

$$\frac{\alpha_0}{\beta_0} = \epsilon_F. \tag{46}$$

Similarly, Eqs. (21a), (45b), and (46) give the other saddle-point condition

$$E - E_0 = \frac{\pi^2 g_0}{6\beta_0^2}. \tag{47}$$

Returning to the state-density formula, Eq. (22), and using Eqs. (44), (46), and (47) we calculate the entropy

$$\begin{aligned}S &\equiv \ln Z(\alpha_0,\beta_0) - \alpha_0 A + \beta_0 E\\ &= \alpha_0 A - \beta_0 E_0 + \frac{g_0\pi^2}{6\beta_0} - \alpha_0 A + \beta_0 E\\ &= \frac{g_0\pi^2}{6\beta_0} + \beta_0(E-E_0)\\ &= \frac{g_0\pi^2}{3\beta_0}.\end{aligned} \tag{48}$$

It is customary to define the excitation energy U relative to the ground-state energy, and the level-density parameter a

$$\begin{aligned}U &\equiv E - E_0 = \frac{\pi^2 g_0}{6\beta_0^2}\\ a &\equiv \frac{\pi^2 g_0}{6},\end{aligned} \tag{49}$$

then the entropy in Eq. (48) can be written

$$S = 2\sqrt{aU}. \tag{50}$$

The second-order partials can be calculated using Eq. (45). The denominator in Eq. (22) reduces to

$$\begin{aligned} 2\pi\sqrt{D}\Big|_{\alpha=\alpha_0,\beta=\beta_0} &= \frac{\pi^2 g_0^2}{3\beta_0^4} \\ &= 4\sqrt{3}U. \end{aligned} \tag{51}$$

Thus we obtain the familiar Fermi-gas state density formula [13]

$$w(A, U) \approx \frac{e^{2\sqrt{aU}}}{4\sqrt{3}U} \tag{52}$$

5. *More sophisticated nuclear models*

The state density given by Eq. (52) can be made more realistic e.g., by including pairing correlations, by treating protons and neutrons as distinguishable particles, etc. (see appendix D.) We will not explore these variations in detail within this paper, because Eq. (52) embodies the essential dependence of the state density as a function of excitation energy, which we will need to calculate explicit forms of the collective enhancement factors. For example, if protons and neutrons are treated as separate particles [11], the exponential dependence $\exp(2\sqrt{aU})$ is unaffected, but the dependence on energy in the denominator changes to $U^{5/4}$. For sufficiently-high excitation energies, the behavior of the state density is almost entirely determined by the exponential behavior, with very little effect from the power-law dependence on U in the denominator.

III. COUNTING LEVELS IN ROTATIONAL NUCLEI

The state and level densities calculated in section II are appropriate for spherical nuclei. If the nucleus is deformed, it will rotate, and new excited levels will appear that cannot be described as intrinsic configurations of the nucleus. The Hamiltonian for the rotating system can be decomposed into three parts,

$$H = H_i + H_r + H_c \tag{53}$$

where H_i is associated with intrinsic excitations of the nucleus (i.e., of the type that were counted in section II), H_r gives rise to rotational levels (not counted by the formalism in section II), and H_c expresses the coupling between intrinsic and rotational motion. The low-lying excitations of a rotating nucleus normally correspond to an adiabatic regime where the motion of the individual nucleons is fast compared to the rotational motion. In the adiabatic regime, the internal configuration of the nucleus is not destroyed by the rotational motion, and the intrinsic and rotational motions can be treated as independent (in other words, H_c can be neglected in Eq. (53)). In this situation, a set of rotational levels (i.e., a band) is built on top of each intrinsic excitation (i.e., the band head). Conversely, if the rotational frequency is too high, the individual nucleons can't "keep up" with the rotational motion, and the separation between intrinsic and rotational motions breaks down (i.e., H_c can no longer be neglected in Eq. (53)).

In principle, the question of obtaining the level density for a rotational nucleus could be solved by writing the Hamiltonian in Eq. (53) explicitly, diagonalizing it in some appropriate basis, and directly counting the levels in a given energy bin. In practice however, except for a few special cases where the Hamiltonian can be written in a particularly simple form, this can be a daunting task. To keep the problem tractable, we will adopt the following strategy:

1. Instead of trying to completely determine the level density for a rotational nucleus, we can tackle the simpler task of calculating the increase in the level density, attributable specifically to the rotational motion (i.e., the rotational enhancement factor).
2. In cases where the Hamiltonian cannot be expressed in a simple form, we will content ourselves with learning what we can about the number of rotational levels based on the structure (i.e., the symmetries) of the Hamiltonian.

With these points in mind, we begin with a study of the use of symmetries as a tool for counting levels.

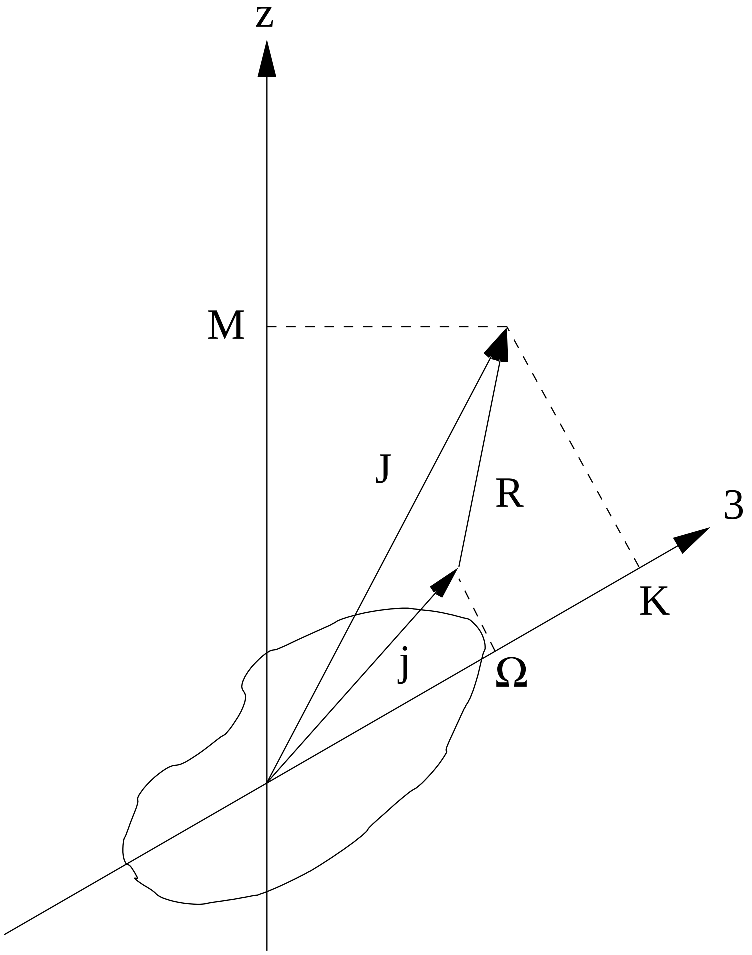

FIG. 1: Definition of laboratory and body-fixed reference frames.

A. Nucleus with no intrinsic symmetries

Consider a generic, unremarkable nuclear shape. We can imagine that, for such a shape, no transformation (e.g., reflection, rotation, etc.) leaves the shape unchanged. This quantum object has no intrinsic symmetries. In more precise terms, there are no transformations (except of course for the identity transformation) which leave the wave functions of the nucleus unchanged.

Because it is a deformed quantum system, such an object must rotate. Therefore, we can identify an intrinsic spin $\vec{j}$, associated with the coupling of individual nucleon spins, a rotational spin $\vec{R}$, associated with the rotational motion of the nucleus as a whole, and a total spin $\vec{J}$ (see Fig. 1) given by

$$\vec{J} = \vec{j} + \vec{R}. \tag{54}$$

We can choose an arbitrary axis, call it the "z axis" in the laboratory frame, and the total spin projection on the z axis, M, will be quantized according to $M = -J, -J+1, \dots, J$. We can also imagine a coordinate system fixed to the rotating body, and label the axes as "1,2,3" to avoid confusion with the laboratory axes "x,y,z". We will call the projection of the total spin $\vec{J}$ on the 3-axis K. The projection of the intrinsic spin $\vec{j}$ on the 3-axis is usually labeled Ω. When the nucleus has no intrinsic symmetries, there are no constraints on the rotational motion other than those imposed by Eq. (54) on the vector $\vec{R}$. As a result, for a given total spin $\vec{J}$ and a given projection M on the laboratory z-axis, its projection K on the body-fixed 3-axis is free to take on any of the values allowed by the quantization of the spin: $K = -J, -J+1, \dots, J$. In other words, to each state defined by $\vec{J}$ and M, there correspond $(2J+1)$ rotational levels.

From a different point of view, we can say that for a nucleus with no intrinsic symmetries and total spin $\vec{J}$, the rotational motion will give rise to $(2J+1)$ levels, each of which contains a $(2J+1)$-fold degeneracy (because of the quantum number M). This is the maximum number of levels we can expect to generate from th rotational motion of the nucleus, for a given total spin J. If we impose additional constraints on the nucleus (in the form of symmetries of the Hamiltonian), the observed number of levels will be reduced. The effect of symmetries on the number of levels is discussed in the examples that follow. To do this we will introduce basic concepts in group theory and illustrate them for some nuclear symmetries of interest.

B. Imposing ellipsoidal symmetry

Consider a rotational Hamiltonian (i.e., the term H_r in Eq. (54)) which is invariant under rotations by angle π about any one of the three body-fixed axes. We can denote these "two-fold"[48] rotations by the symbols $C_2^{(i)}$, where the superscript $i = 1, 2, 3$ indicates the axis of rotation in the body frame. The three rotations $C_2^{(1)}$, $C_2^{(2)}$, $C_2^{(3)}$, along with the identity operator, E, form a group in the mathematical sense. This particular group is commonly denoted by the symbol D_2, the group of ellipsoidal symmetry. As with all groups its elements $C_2^{(1)}$, $C_2^{(2)}$, $C_2^{(3)}$, and E satisfy the four properties that define a mathematical group [14]

1. The product of two elements of the group is also an element of the group: this closure property can be proved in the case of the C_2 operators by considering the effect of each operator on a point (x_1, x_2, x_3) in the 3-body frame:

$$\begin{aligned} E:\ & (x_1,x_2,x_3) \to (x_1,x_2,x_3) \\ C_2^{(1)}:\ & (x_1,x_2,x_3) \to (x_1,-x_2,-x_3) \\ C_2^{(2)}:\ & (x_1,x_2,x_3) \to (-x_1,x_2,-x_3) \\ C_2^{(3)}:\ & (x_1,x_2,x_3) \to (-x_1,-x_2,x_3). \end{aligned}$$

   Then, for example, if we compose the rotations about the 1-axis and 2-axis, we can write

$$\begin{aligned} C_2^{(1)}C_2^{(2)} : (x_1,x_2,x_3) \xrightarrow{C_2^{(2)}} (-x_1,x_2,-x_3) \xrightarrow{C_2^{(1)}} & (-x_1,-x_2,-(-x_3)) \\ = & (-x_1,-x_2,x_3), \end{aligned}$$

   which is just the effect of the $C_2^{(3)}$ operator. If we consider all the possible products, we construct Table I, which proves closure.

TABLE I: Tabulated binary products of the operators of the group D_2.

	E	$C_2^{(1)}$	$C_2^{(2)}$	$C_2^{(3)}$
E	E	$C_2^{(1)}$	$C_2^{(2)}$	$C_2^{(3)}$
$C_2^{(1)}$	$C_2^{(1)}$	E	$C_2^{(3)}$	$C_2^{(2)}$
$C_2^{(2)}$	$C_2^{(2)}$	$C_2^{(3)}$	E	$C_2^{(1)}$
$C_2^{(3)}$	$C_2^{(3)}$	$C_2^{(2)}$	$C_2^{(1)}$	E

2. The product of two elements of the group is associative: This property could also be verified exhaustively for products of any three elements, thus for example

$$\begin{aligned} \left(C_2^{(1)}C_2^{(2)}\right)C_2^{(2)} &= C_2^{(3)}C_2^{(2)} \\ &= C_2^{(1)}, \end{aligned}$$

   where we've used the product table in property 1. Likewise we can calculate this product as

$$\begin{aligned} C_2^{(1)}\left(C_2^{(2)}C_2^{(2)}\right) &= C_2^{(1)}E \\ &= C_2^{(1)}, \end{aligned}$$

   which is the same result, as required by associativity.

3. The group contains a unit element: in this case, we've explicitly included the operator E.
4. The inverse of each element of the group is contained within the group: this can be seen by looking at the diagonal of Table I, i.e., each element of D_2 is its own inverse.

What we have not made clear so far is what has been gained by noting that the symmetry-preserving transformations $C_2^{(1)}$, $C_2^{(2)}$, $C_2^{(3)}$, and E form a group. In fact we will show that *the fact that the Hamiltonian is not affected by the four elements of the group D_2 directly implies that only a fourth of its eigenvalues for a given total spin $\vec{J}$ will be observed.* This is a powerful statement we can make about the number of levels without ever writing down an explicit form for the Hamiltonian. However, the validity of this statement is not immediately obvious. But before we discuss the usefulness of mathematical groups, we need to understand what is actually meant by the concept of invariance in the present context.

Consider a basis $|u\rangle$, which is transformed into a new basis $|u'\rangle$ by an operator T, i.e.,

$$|u\rangle \xrightarrow{T} |u'\rangle \equiv T\,|u\rangle\,. \tag{55}$$

We wish to know how the operator T will transform an operator M into the new basis. For this, we use the definition in Eq. (55),

$$\begin{aligned} M\,|u\rangle &\xrightarrow{T} TM\,|u\rangle \\ &= TMT^{-1}\,|u'\rangle\,, \end{aligned} \tag{56}$$

where T^{-1} is the inverse operator of T.

Now consider the Hamiltonian operator H, and suppose that it is invariant under some symmetry transform T. This invariance property can be written explicitly as

$$\begin{aligned} &H = THT^{-1} \\ \Rightarrow\;\; &[H,T] \equiv HT - TH = 0. \end{aligned} \tag{57}$$

In other words, saying that the Hamiltonian is invariant under a symmetry operation is equivalent to saying that the Hamiltonian operator commutes with the symmetry operator.

It is well known in quantum mechanics (see, e.g., [15]) that when two operators commute, they share a common basis. We will show that if we can make statements about the "structure" of the symmetry operators in the common basis, the same statements will apply to the Hamiltonian operator they commute with. To clarify what we mean by this, consider a Hamiltonian H, a symmetry operator T for this Hamiltonian, and a basis $|u\rangle$ common to both operator. Suppose we discover that the kets $|u\rangle$ fall into two categories,$|u^{(1)}\rangle$ and $|u^{(2)}\rangle$, with respect to the operator T, based on the corresponding eigenvalues. (There is nothing special about the number two in this case, more categories may exist, but two is simplest for illustrative purposes.) Thus we assume in our example that the kets $|u^{(1)}\rangle$ have eigenvalue u_1, while the kets $|u^{(2)}\rangle$ have a different eigenvalue u_2

$$\begin{aligned} T\,|u^{(1)}\rangle &= u_1\,|u^{(1)}\rangle \\ T\,|u^{(2)}\rangle &= u_2\,|u^{(2)}\rangle\,, \end{aligned} \tag{58}$$

where $u_1 \neq u_2$, and where we will assume that both u_1 and u_2 are real to avoid cumbersome notation. Then we can draw a remarkable conclusion about the Hamiltonian. Indeed, consider the matrix element of the commutator in Eq. (57) between the two categories of basis states

$$\begin{aligned} [H,T] = 0 \;\Rightarrow\; &\left\langle u^{(2)} \middle| [H,T] \middle| u^{(1)} \right\rangle = 0 \\ \Rightarrow\; &\left\langle u^{(2)} \middle| HT - TH \middle| u^{(1)} \right\rangle = 0 \\ \Rightarrow\; &\left\langle u^{(2)} \middle| HT \middle| u^{(1)} \right\rangle - \left\langle u^{(2)} \middle| TH \middle| u^{(1)} \right\rangle = 0 \\ \Rightarrow\; &(u_1 - u_2)\left\langle u^{(2)} \middle| H \middle| u^{(1)} \right\rangle = 0. \end{aligned} \tag{59}$$

Because we assumed $u_1 \neq u_2$, it follows that the off-diagonal matrix element $\langle u^{(2)} | H | u^{(1)} \rangle$ must be zero. This means we have identified two categories of basis states which are not connected by the Hamiltonian of the system. Experimentally, we will only observe eigenstates of Hamiltonian expressed in terms of the basis states $|u^{(1)}\rangle$ or the basis states $|u^{(2)}\rangle$, but not both. Therefore, fewer eigenstates will be observed than if we could access the full $|u\rangle$ basis.

We will show that this is precisely what happens in the case of the rotational Hamiltonian with D_2 symmetry [16]. In general, the wave function of a rotational nucleus, characterized by total angular momentum $\vec{J}$ and projection M on the laboratory z-axis, can be written as a linear combination of many states with well-defined projection K on the 3-axis of the body-fixed frame

$$|JM\rangle = \sum_{K=-J}^{J} a_K^J \, |JMK\rangle \,, \tag{60}$$

where the a_K^J are coefficients of the expansion. In order to make statements about the invariance of the $|JM\rangle$ wave function under D_2 symmetry, we need to know how the kets $|JMK\rangle$ are transformed by the group operators $C_2^{(1)}$, $C_2^{(2)}$, $C_2^{(3)}$, and E. The effect of the identity operator is trivial

$$E \, |JMK\rangle = |JMK\rangle \,. \tag{61}$$

Calculating the effect of the two-fold rotations on the $|JMK\rangle$ kets requires more work. It is helpful to introduce the concept of a general rotation in quantum mechanics. This is done in many standard texts and articles (see,e.g., [17–20]). The rotation of a coordinate system in quantum mechanics, as in classical mechanics, is often expressed in terms of Euler angles [21]. Any rotation of the coordinate axes can then be effected by applying the following algorithm [18]

1. Rotate through θ_1 about the z-axis.
2. Rotate through θ_2 about the new y-axis.
3. Rotate through θ_3 about the new z-axis.

The Euler angles cover the range $0 \leq \theta_i < 2\pi$, with $i = 1, 2, 3$. The corresponding rotation operator $R(\theta_1, \theta_2, \theta_3)$ for the body-fixed frame can be written in terms of the components of the angular-momentum operator $\hat{J}_1$, $\hat{J}_2$, $\hat{J}_3$ along the three axes by following the algorithm above

$$R(\theta_1, \theta_2, \theta_3) = e^{-i\theta_1 \hat{J}_3} e^{-i\theta_2 \hat{J}_2} e^{-i\theta_3 \hat{J}_3} . \tag{62}$$

It can be shown [22] that the operators $\hat{J}_1$, $\hat{J}_2$, $\hat{J}_3$ satisfy the commutation relations

$$\begin{aligned} \left[\hat{J}_1, \hat{J}_2\right] &= -\hbar i \hat{J}_3 \\ \left[\hat{J}_2, \hat{J}_3\right] &= -\hbar i \hat{J}_1 \\ \left[\hat{J}_3, \hat{J}_1\right] &= -\hbar i \hat{J}_2 . \end{aligned} \tag{63}$$

Note the these commutation relations have the opposite sign to the familiar commutation relation for angular-momentum operators in the laboratory frame. The appearance of the minus sign in Eq. (63) can be traced to the fact that the rotations generated by the components $\hat{J}_1$, $\hat{J}_2$, $\hat{J}_3$ actually modify the body-fixed coordinate system, whereas the corresponding laboratory-frame components $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$ rotate the nucleus itself.

To investigate the effect of the coordinate-rotation on the vector $|JK\rangle$, we write

$$R(\theta_1, \theta_2, \theta_3) \, |JK\rangle = \sum_{K'=-J}^{J} |JK'\rangle \, \langle JK' | R(\theta_1, \theta_2, \theta_3) | JK\rangle \,, \tag{64}$$

where we've inserted a complete set of states on the right-hand side. The matrix elements $\langle JK' | R(\theta_1, \theta_2, \theta_3) | JK\rangle$ are the well-known [18] Wigner D functions, denoted by

$$D^J_{K'K}(\theta_1,\theta_2,\theta_3) \equiv \langle JK'|R(\theta_1,\theta_2,\theta_3)|JK\rangle\,. \tag{65}$$

The two-fold rotation about the 3-axis, $C_2^{(3)}$, can be described simply in terms of the Euler angles $\theta_1 = \pi$, $\theta_2 = 0$, and $\theta_3 = 0$. The corresponding matrix element is

$$\begin{aligned} D^J_{K'K}(\pi,0,0) &= \left\langle JK'\middle|e^{-i\pi\hat{J}_3}e^{-i\times 0\times\hat{J}_2}e^{-i\times 0\times\hat{J}_3}\middle|JK\right\rangle \\ &= \left\langle JK'\middle|e^{-i\pi\hat{J}_3}\middle|JK\right\rangle \\ &= e^{-i\pi K}\delta_{K,K'}\,, \end{aligned} \tag{66}$$

where we've used $\hat{J}_3\,|JK\rangle = K\,|JK\rangle$, and the Taylor expansion for the exponential function of an operator in the last step. Using this result in Eq. (64), we write, for the kets $|JMK\rangle$ in Eq. (60),

$$\begin{aligned} C_2^{(3)}\,|JMK\rangle &= R(\pi,0,0)\,|JMK\rangle \\ &= \sum_{K'=-J}^{J} D^J_{K'K}(\pi,0,0)\,|JMK'\rangle \\ &= \sum_{K'=-J}^{J} e^{-i\pi K}\delta_{K,K'}\,|JMK'\rangle \\ &= e^{-i\pi K}\,|JMK\rangle\,. \end{aligned} \tag{67}$$

We can proceed in a similar manner to calculate the effect of the two-fold rotation about the 2-axis, $C_2^{(2)}$, on $|JMK\rangle$

$$\begin{aligned} C_2^{(2)}\,|JMK\rangle &= R(0,\pi,0)\,|JMK\rangle \\ &= \sum_{K'=-J}^{J} D^J_{K'K}(0,\pi,0)\,|JMK'\rangle\,. \end{aligned} \tag{68}$$

The Wigner D functions have been extensively studied, and we can calculate them using a general explicit formula [22]

$$D^J_{K'K}(0,\pi,0) = (-1)^{J+K'}\delta_{K,-K'}\,. \tag{69}$$

With a bit of work, it is possible to derive this result. The derivation itself calls upon ideas and techniques that are useful in their own right and is discussed in appendix B. Using Eq. (69), we simplify Eq. (68)

$$\begin{aligned} C_2^{(2)}\,|JMK\rangle &= \sum_{K'=-J}^{J} (-1)^{J+K'}\delta_{K,-K'}\,|JMK'\rangle \\ &= (-1)^{J-K}\,|JM,-K\rangle\,. \end{aligned} \tag{70}$$

Finally, to obtain the effect of the two-fold rotation about the 1-axis, with as little effort as possible, we remember that $C_2^{(1)} = C_2^{(2)}C_2^{(3)}$, according to Table I. Thus, using Eqs. (67) and (70), we write

$$\begin{aligned} C_2^{(1)}\,|JMK\rangle &= C_2^{(2)}C_2^{(3)}\,|JMK\rangle \\ &= (-1)^{J-K}(-1)^K\,|JM,-K\rangle \\ &= (-1)^J\,|JM,-K\rangle\,. \end{aligned} \tag{71}$$

In deriving Eqs. (67), (70), and (71) we have tacitly assumed that J (and therefore K) is an integer. Without this assumption, the group structure would have been more complicated (see, e.g., [23]), and we could not have simplified the exponential expressions in the equations above as we did. Clearly, Eqs. (67), (70), and (71) show that the kets $|JMK\rangle$ are not eigenfunctions of all the D_2 operators. However, we can define a new basis with symmetric states

$$|JMK\rangle_S \equiv \begin{cases} \frac{1}{\sqrt{2}}\left(|JMK\rangle + |JM,-K\rangle\right) & K \neq 0 \\ |JM0\rangle & K = 0, \end{cases} \tag{72}$$

and anti-symmetric basis states

$$|JMK\rangle_A \equiv \frac{1}{\sqrt{2}}\left(|JMK\rangle - |JM,-K\rangle\right) \qquad K \neq 0, \tag{73}$$

that are eigenfunctions of the operators E, $C_2^{(1)}$, $C_2^{(2)}$, and $C_2^{(3)}$. (Note that there is no anti-symmetric state with $K = 0$ in Eq. (73) since, by definition, $|JM0\rangle_A = (|JM0\rangle - |JM,0\rangle)/\sqrt{2} = 0$, the null vector.) We list the eigenvalues that correspond to the four D_2 operators in Table II.

TABLE II: Tabulated eigenvalues of the D_2 operators on the symmetric and anti-symmetric basis kets

	E	$C_2^{(1)}$	$C_2^{(2)}$	$C_2^{(3)}$
$\lvert JMK\rangle_S$ [a]	1	$(-1)^{J-K}$	$(-1)^J$	$(-1)^K$
$\lvert JM0\rangle_S$	1	$(-1)^J$	$(-1)^J$	1
$\lvert JMK\rangle_A$ [a]	1	$-(-1)^{J-K}$	$-(-1)^J$	$(-1)^K$

[a] $K \neq 0$

The eigenvalues in Table II suggest different categories, based on the parity of J, K, and the symmetry of the kets. Thus, if we define the quantity

$$\gamma \equiv \begin{cases} 0 & \text{for symmetric kets} \\ 1 & \text{for anti-symmetric kets} \end{cases} \tag{74}$$

for convenience, we can construct the classification in Table III. Table III is commonly referred to as a "character table", and the set of eigenvalues in each row correspond to a particular "representation" of the group. These representations are labeled by the symbols A, B_1, B_2, B_3. These symbols are not arbitrarily chosen, they are called Mulliken symbols, and have a precise meaning which we will not discuss here (see, e.g., [24, 25]).

TABLE III: Classification of the nuclear states into "representations", according to the effect of the D_2 operators. The last column gives a label for each representation

Description	E	$C_2^{(1)}$	$C_2^{(2)}$	$C_2^{(3)}$	Label
$J+\gamma$ = even, K = even	1	1	1	1	A
$J+\gamma$ = odd, K = odd	1	1	-1	-1	B_1
$J+\gamma$ = even, K = odd	1	-1	1	-1	B_2
$J+\gamma$ = odd, K = even	1	-1	-1	1	B_3

We can show that the matrix elements of the Hamiltonian between basis states in different representations are identically zero, as we showed in Eq. (59). Thus, for example, if we let $|A\rangle$ stand for a state in representation A, and $|B_1\rangle$ stand for a state in representation B_1, we can take advantage of the fact that that Hamiltonian H is invariant under the operator $C_2^{(2)}$ to write

$$\begin{aligned} \left[H, C_2^{(2)}\right] = 0 \;&\Rightarrow\; \left\langle B_1 \middle| \left[H, C_2^{(2)}\right] \middle| A \right\rangle = 0 \\ &\Rightarrow\; \left\langle B_1 \middle| H C_2^{(2)} - C_2^{(2)} H \middle| A \right\rangle = 0 \\ &\Rightarrow\; \left\langle B_1 \middle| H C_2^{(2)} H \middle| A \right\rangle - \left\langle B_1 \middle| C_2^{(2)} H \middle| A \right\rangle = 0 \\ &\Rightarrow\; 2 \langle B_1 | H | A \rangle = 0, \end{aligned} \tag{75}$$

where we've used the results in Table III. Clearly, Eq. (75) implies that $\langle B_1|H|A\rangle = 0$, i.e., that states constructed from the basis kets in representation A are not connected to those generated in representation B_1. The same can be show for any pair of distinct representations in Table III, by choosing any one of the four D_2 operators that has different eigenvalues in the two representations.

Experimentally, we will only observe those states that are associated with one of the representations, but not the three other (since the off-diagonal matrix elements of H are zero, there is no mechanism for making a transition from one representation to another). The remaining question is: which of the four representations will be seen experimentally?

We can best answer this question by looking at the experimental evidence for "triaxial" rotors (i.e. rotors with three distinct moments of inertia, but overall D_2 symmetry). Low-lying triaxial levels in even-even nuclei include a 0^+ ground state. A careful examination of Table III reveals that only one representation contains a $J = 0$ state, the A representation. This is because $J = 0 \Rightarrow K = 0$, which rules out the representations with $K =$ odd (i.e., B_1 and B_2), and for representation B_3, $J + \gamma =$ odd means that $\gamma = 1$, which refers to the anti-symmetric kets $|JMK\rangle_A$, and we have already argued that $K = 0$ is not allowed for those states.

The final task at hand is to count the number of states than can be constructed in each of the four D_2 representations. This can be done using Table III. To illustrate the process, we use the following examples

Example 1. *Count the number of states in each representation in Table III for the total spin $J = 4$.*

Rep. A

$$\left.\begin{array}{l} J+\gamma = \text{even} \Rightarrow \gamma = 0 \text{ (i.e., symmetric)} \\ K = \text{even} \end{array}\right\} \Rightarrow K = 0, 2, 4 \tag{76}$$

Rep. B_1

$$\left.\begin{array}{l} J+\gamma = \text{odd} \Rightarrow \gamma = 1 \text{ (i.e., anti-symmetric)} \\ K = \text{odd} \end{array}\right\} \Rightarrow K = 1, 3 \tag{77}$$

Rep. B_2

$$\left.\begin{array}{l} J+\gamma = \text{even} \Rightarrow \gamma = 0 \text{ (i.e., symmetric)} \\ K = \text{odd} \end{array}\right\} \Rightarrow K = 1, 3 \tag{78}$$

Rep. B_3

$$\left.\begin{array}{l} J+\gamma = \text{odd} \Rightarrow \gamma = 1 \text{ (i.e., anti-symmetric)} \\ K = \text{even} \end{array}\right\} \Rightarrow K = 2, 4 \tag{79}$$

Note that the $K = 0$ case is discarded because of the assumption of anti-symmetric kets.

Example 2. *Count the number of states in each representation for the total spin $J = 5$.*

Rep. A

$$\left.\begin{array}{l} J+\gamma = \text{even} \Rightarrow \gamma = 1 \text{ (i.e., anti-symmetric)} \\ K = \text{even} \end{array}\right\} \Rightarrow K = 2, 4 \tag{80}$$

Note that the $K = 0$ case is discarded because of the assumption of anti-symmetric kets.

Rep. B_1

$$\left.\begin{array}{l} J+\gamma = \text{odd} \Rightarrow \gamma = 0 \text{ (i.e., symmetric)} \\ K = \text{odd} \end{array}\right\} \Rightarrow K = 1, 3, 5 \tag{81}$$

Rep. B_2

$$\left.\begin{array}{l} J+\gamma = \text{even} \Rightarrow \gamma = 1 \text{ (i.e., anti-symmetric)} \\ K = \text{odd} \end{array}\right\} \Rightarrow K = 1, 3, 5 \tag{82}$$

TABLE IV: Number of levels in each representation of D_2 for a given total angular momentum J of integer value.

	A	B_1, B_2, B_3
J even	$\frac{1}{2}J+1$	$\frac{1}{2}J$
J odd	$\frac{1}{2}J-\frac{1}{2}$	$\frac{1}{2}J+\frac{1}{2}$

Rep. B_3

$$\left.\begin{array}{l} J+\gamma = \text{odd} \Rightarrow \gamma = 0 \text{ (i.e., symmetric)} \\ K = \text{even} \end{array}\right\} \Rightarrow K = 0, 2, 4 \tag{83}$$

We can generalize these examples and produce Table IV of the number of levels, for a given total spin J, in each representation [16].

From Table IV we see that the $(2J+1)$ states of a nucleus without intrinsic symmetries (see section III A) are divided approximately evenly between the four representations, hence the fourfold decrease in level density produced by the imposition of D_2 symmetry [2].

C. Imposing reflection symmetry

Another symmetry commonly encountered in nuclei, is reflection symmetry. This corresponds to invariance under reflection about a plane. In particular, if we consider the reflection about a plane perpendicular to the 3-axis, the reflection operator is denoted by the symbol σ_h, where the subscript "h" indicates a "horizontal" plane. The operation σ_h, along with the identity operator E form a group, in the sense of the group properties 1 – 4 in section III B. This two-element group is denoted by the Schoenflies symbol "C_S", and is sometimes referred to as a "monoclinic" point group in the literature [26, 27].

The effect of the group operators, E and σ_h on the kets $|JMK\rangle$ is simply

$$\begin{aligned} E\,|JMK\rangle &= |JMK\rangle \\ \sigma_h\,|JMK\rangle &= |JM,-K\rangle \end{aligned} \tag{84}$$

and the kets $|JMK\rangle$ are not eigenfunctions of the reflection operator. However, if we consider the symmetric and anti-symmetric basis kets defined in Eqs. (72) and (73), respectively, we find that they are eigenfunctions of both E and σ_h. If we divide the complete basis into symmetric kets, which we associate with a representation A', and anti-symmetric kets, associated with the representation A'', we construct the character table, Table V.

TABLE V: Character table for the C_S group

	E	σ_h
A'	1	1
A''	1	-1

From the character table, we see that the C_S symmetry divides the observed levels into the two representations A' and A''. For a given total angular momentum, there are $J+1$ states in the A' representation, corresponding to the symmetric-ket basis with $K = 0, 1, 2, \ldots, J$, and J states in the A'' representation, corresponding to the anti-symmetric-ket basis with $K = 1, 2, \ldots, J$. Experimentally, we observe the states in one representation or the other, but not both (see the discussion in section III B). Thus, the level density decreases by a factor of $\approx 1/2$.

Conversely, if a system violates reflection symmetry, the full basis of symmetric and anti-symmetric kets becomes available, and the level density increases by a factor of two. Nuclei with octupole deformation (i.e., "pear"-shapes, "banana"-shapes, etc. [28, 29]) are reflection-asymmetric, and a doubling of the level density can be expected, relative to a nucleus that respects the C_S symmetry.

D. Axially-symmetric nuclei

1. *Group-theoretical treatment*

Axially-symmetric shapes, also referred to as symmetric tops, belong to the D_∞ symmetry group, which is the group of rotations about a special axis (the symmetry axis) through any angle $0 \le \phi < 2\pi$, and rotations by π about any axis perpendicular to the symmetry axis (and not just about the 1- and 2-axes) [23]. By convention, we take the 3-axis as the symmetry axis of the nucleus.

As with the analysis of ellipsoidal and reflection symmetries in sections III B and III C, respectively, we can learn a great deal about the levels of an axially-symmetric rotor simply by examining its symmetries. The elements of the point group D_∞ are the identity operator E, the rotation operator $C_\phi^{(3)}$ about the 3-axis through the angle ϕ, and the twofold rotation C_2 about an arbitrary axis perpendicular to the 3-axis. The identity operator leaves a ket $|JMK\rangle$ unchanged

$$E\,|JMK\rangle = |JMK\rangle\,. \tag{85}$$

The effect of the operator $C_\phi^{(3)}$ can be calculated in straightforward way (see the discussion of rotation operators in section III B)

$$\begin{aligned} C_\phi^{(3)}\,|JMK\rangle &= e^{-i\phi\hat{J}_3}\,|JMK\rangle \\ &= e^{-i\phi K}\,|JMK\rangle\,, \end{aligned} \tag{86}$$

which is simply a generalization of Eq. (67). The effect of the operator C_2 in this case requires a bit more work to calculate. The result of rotating the body-fixed coordinate system by π about an axis perpendicular to the 3-axis can be obtained, for example, by rotating by some arbitrary angle α about the 3-axis, and then rotating by π about the new 2-axis. We write

$$\begin{aligned} C_2\,|JMK\rangle &= e^{-i\pi\hat{J}_2}e^{-i\alpha\hat{J}_3}\,|JMK\rangle \\ &= e^{-i\pi\hat{J}_2}e^{-i\alpha K}\,|JMK\rangle \\ &= e^{-i\alpha K}(-1)^{J-K}\,|JM,-K\rangle\,, \end{aligned} \tag{87}$$

where we've used Eq. (70) in the last step. For a given total angular momentum J, we have $K = -J, -J+1, \ldots, J$, and we are free to order the kets $|JMK\rangle$ arbitrarily in the basis. In particular, we choose the order

$$|JM0\rangle\,, |JM,-1\rangle\,, |JM1\rangle\,, \ldots, |JM,-J\rangle\,, |JMJ\rangle \tag{88}$$

that is, we group together the kets with opposite signs of K. In this re-ordered basis, the matrix representation of the D_∞ group operators [49] can be written using Eqs. (85), (86), and (87)

$$D(E) = \begin{pmatrix} 1 & \cdots & & & & \\ \vdots & 1 & 0 & & & \\ & 0 & 1 & & & \\ & & & \ddots & & \\ & & & & 1 & 0 \\ & & & & 0 & 1 \end{pmatrix}, \tag{89}$$

where $D(E)$ is the matrix representation of the identity operator E, and where the unwritten matrix elements are equal to zero. The matrix representation of $C_\phi^{(3)}$ is

$$D(C_\phi^{(3)}) = \begin{pmatrix} 1 & \cdots & & & & \\ \vdots & e^{i\phi} & 0 & & & \\ & 0 & e^{-i\phi} & & & \\ & & & \ddots & & \\ & & & & e^{iJ\phi} & 0 \\ & & & & 0 & e^{-iJ\phi} \end{pmatrix}, \tag{90}$$

and for the operator C_2 we write the matrix

$$D(C_2) = \begin{pmatrix} (-1)^J & \cdots & & & & \\ \vdots & 0 & (-1)^{J+1}e^{i\phi} & & & \\ & (-1)^{J-1}e^{-i\phi} & 0 & & & \\ & & & \ddots & & \\ & & & & 0 & e^{iJ\phi} \\ & & & & e^{-iJ\phi} & 0 \end{pmatrix}. \tag{91}$$

We have written the matrix representations in Eqs. (89), (90) and (91) explicitly to emphasize their common structure, namely the block diagonal form,

$$\begin{pmatrix} X & \cdots & & & & \\ \vdots & X & X & & & \\ & X & X & & & \\ & & & \ddots & & \\ & & & & X & X \\ & & & & X & X \end{pmatrix}, \tag{92}$$

where the symbols X stand for matrix elements that are not necessarily zero. In fact, we can show that the structure of the D_∞ matrices cannot be reduced to a form simpler than that of Eq. (92), i.e., the two-dimensional blocks cannot be diagonalized further for all the group elements simultaneously. To prove this, we choose a generic block, corresponding to a specific value of K, and generated from the sub-basis $\{|JM,-K\rangle, |JMK\rangle\}$. For $K \neq 0$, the sub-matrices are

$$\begin{aligned} D_K(E) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, D_K\left(C_\phi^{(3)}\right) = \begin{pmatrix} e^{iK\phi} & 0 \\ 0 & e^{-iK\phi} \end{pmatrix}, \\ D_K(C_2) &= \begin{pmatrix} 0 & (-1)^{J+K}e^{i\alpha K} \\ (-1)^{J-K}e^{-i\alpha K} & 0 \end{pmatrix} \end{aligned} \tag{93}$$

We want to show that no linear combination of the sub-basis kets can be formed which is a simultaneous eigenfunction of $D_K(E)$, $D_K(C_\phi^{(3)})$, and $D_K(C_2)$. This will show that the sub-basis $\{|JM,-K\rangle, |JMK\rangle\}$ cannot be transformed into a new sub-basis where the two-dimensional blocks in Eq. (89), (90), and (91) can be diagonalized, and therefore reduced to two one-dimensional blocks. We first assume that such a sub-basis exists, and that each of its elements

$$|u_i\rangle \equiv a_i |JM,-K\rangle + b_i |JMK\rangle, \tag{94}$$

is an eigenfunction of $D_K(E)$, $D_K(C_\phi^{(3)})$, and $D_K(C_2)$. We will now try to determine the coefficients a_i and b_i. The ket $|u_i\rangle$ is always an eigenstate of the identity operator, no matter what the values of a_i and b_i. We apply the other two matrix operations

$$D_K(C_\phi^{(3)}) |u_i\rangle = a_i e^{iK\phi} |JM,-K\rangle + b_i e^{-iK\phi} |JMK\rangle. \tag{95}$$

If we require that this is an eigenstate of $D_K(C_\phi^{(3)})$ with some eigenvalue λ_1 then we must have

$$D_K(C_\phi^{(3)})\left|u_i\right\rangle = \lambda_1 \left|u_i\right\rangle \Rightarrow \left\{ \begin{array}{c} a_i e^{iK\phi} = \lambda_1 a_i \\ b_i e^{-iK\phi} = \lambda_1 b_i \end{array} \right. . \tag{96}$$

Similarly,

$$D_K(C_2)\left|u_i\right\rangle = a_i(-1)^{J+K} e^{i\alpha K}\left|JMK\right\rangle + b_i(-1)^{J-K} e^{-i\alpha K}\left|JM,-K\right\rangle, \tag{97}$$

and therefore, for some eigenvalue λ_2,

$$D_K(C_2)\left|u_i\right\rangle = \lambda_2 \left|u_i\right\rangle \Rightarrow \left\{ \begin{array}{c} b_i(-1)^{J-K} e^{-i\alpha K} = \lambda_2 a_i \\ a_i(-1)^{J+K} e^{i\alpha K} = \lambda_2 b_i \end{array} \right. . \tag{98}$$

To understand the implications of Eqs. (96) and (98) for $K \neq 0$, we consider three cases, depending on whether a_i and b_i are zero or not.

1. $a_i = 0$: then Eq. (98) implies that $b_i = 0$ as well. Therefore $\left|u_i\right\rangle = 0$, which means it cannot serve as a basis ket. This is not an acceptable solution.
2. $b_i = 0$: again, by Eq. (98) we conclude that $a_i = 0$ also, and that $\left|u_i\right\rangle = 0$. This solution is also unacceptable.
3. $a_i \neq 0$ and $b_i \neq 0$: in this case, we can simplify Eq. (96) to

$$\left\{ \begin{array}{c} e^{iK\phi} = \lambda_1 \\ e^{-iK\phi} = \lambda_1 \end{array} \right. , \tag{99}$$

which cannot be solved for λ_1, unless $K = 0$.

We conclude that, for $K \neq 0$, the two-dimensional blocks in the matrix representations for E, $C_\phi^{(3)}$, and C_2 cannot be further reduced by any change of basis. We say that the two-dimensional representation formed by the sub-basis $\{\left|JM,-K\right\rangle, \left|JMK\right\rangle\}$ for $K \neq 0$ is *irreducible.* The 1×1 block corresponding to $K = 0$ in each matrix is trivially irreducible. We must emphasize that it is the submatrices $D_K(E)$, $D_K(C_\phi^{(3)})$, and $D_K(C_2)$ that are irreducible, because they cannot be simultaneously brought into the same block-diagonal form by a choice of basis. In contrast, the full matrices $D(E)$, $D(C_\phi^{(3)})$, and $D(C_2)$ are not irreducible because they have the same block structure.

Now we are in a position to apply the tools of group theory to show how the common structure displayed by Eq. (92) can be used to classify and count the levels of the axially-symmetric rotor. The tool that allows us to do this is sometimes referred to as "Schur's lemma" in the literature [25, 30]. Schur's lemma asserts that a matrix which commutes with all the matrices of an irreducible representation must be of the form

$$\begin{pmatrix} \lambda & 0 & \cdots \\ 0 & \lambda & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \tag{100}$$

i.e., a diagonal matrix of the same dimension as the irreducible representation, with a single constant, λ, along the diagonal. A rigorous proof of the lemma is given in [25]. In plain words, the proof proceeds by writing the commutation of a matrix A with the irreducible matrix representations $D(G)$ of all the members of a group G in a basis where the matrix A is diagonalized. In this special basis, the commutation relations can be written in a particularly simple form in terms of the matrix elements of A and $D(G)$. From this result, it becomes clear that if A commutes with all the $D(G)$ matrices then either a) the $D(G)$ matrices have been cast into block-diagonal form by the change of basis, or b) all the elements along the diagonal of A are equal. The former possibility contradicts the initial assumption that the $D(G)$ matrices are irreducible, therefore A must be of the form of Eq. (100).

We can apply Schur's lemma to the problem at hand. The fact that the Hamiltonian commutes with all the elements of the group D_∞ implies that its matrix representation must have the structure of Eq. (92), by arguments similar to those in Eqs. (59) or (75) (these arguments have nothing to do with Schur's lemma because the full matrices are not irreducible, only the submatrices are). For $K \neq 0$, the 2×2 block in the Hamiltonian matrix corresponding to the sub-basis $\{|JM,-K\rangle, |JMK\rangle\}$ commutes with the irreducible representations $D_K(E)$, $D_K(C_\phi^{(3)})$, and $D_K(C_2)$, because of the requirement of invariance with respect to these symmetry operations. By Schur's lemma, this implies that the Hamiltonian is two-fold degenerate for each $K \neq 0$, i.e. of a two-dimensional form of Eq. (100). For $K = 0$, the irreducible representations of the D_∞ elements are 1×1 matrices, therefore a single level is expected in this case.

To further investigate the $K = 0$ case, we note that the matrices in Eqs. (89), (90), and (91) were formulated for a fixed total angular momentum J, and the projection K taking on all possible values from $-J$ to J. We could have have fixed K instead, and allowed J to take all the allowed values. This is a useful if somewhat more difficult approach, because the matrices in that case have infinite dimensions. In the $K = 0$ case in particular, the matrix representations of E and $C_\phi^{(3)}$ would both be the identity matrix, because of Eqs. (85) and (86), respectively. But, according to Eq. (87), the matrix representation of C_2 would be diagonal, with values along the diagonal equal to $+1$ for even J, or -1 for odd J. As a result, the original representation would be reduced to two new representations, defined by the parity of the spin J. Thus, if we classify the even-J states into the representation A_e and the odd-J states into the representation A_o, the fact that C_2 and the Hamiltonian H commute implies

$$\begin{aligned} \langle A_o|HC_2 - C_2H|A_e\rangle &= 0 \\ -\langle A_o|H|A_e\rangle - \langle A_o|H|A_e\rangle &= 0 \\ \langle A_o|H|A_e\rangle &= 0 \end{aligned} \tag{101}$$

where $|A_e\rangle$ and $|A_o\rangle$ stand for any basis ket belonging to the even or odd representations, respectively. Eq. (101) shows that we indeed have two distinct sets of states corresponding to $K = 0$, one set with $J = 0, 2, 4, \ldots$, and the other with $J = 1, 3, 5, \ldots$.

2. Explicit calculation of the level density

The symmetric top is a special case for which the rotational Hamiltonian is particularly simple, and explicit formulas can be obtained for the rotational energies. In this case, the moments of inertia about the 1-axis and 2-axis are equal, $\mathcal{I}_1 = \mathcal{I}_2 \equiv \mathcal{I}$, and the rotational Hamiltonian is [17]

$$\begin{aligned} H_r &= \frac{\hbar^2 \hat{R}_1^2}{2\mathcal{I}_1} + \frac{\hbar^2 \hat{R}_2^2}{2\mathcal{I}_2} + \frac{\hbar^2 \hat{R}_3^2}{2\mathcal{I}_3} \\ &= \frac{\hbar^2 (\hat{R}_1^2 + \hat{R}_2^2)}{2\mathcal{I}} + \frac{\hbar^2 \hat{R}_3^2}{2\mathcal{I}_3} \\ &= \frac{\hbar^2 (\hat{R}^2 - \hat{R}_3^2)}{2\mathcal{I}} + \frac{\hbar^2 \hat{R}_3^2}{2\mathcal{I}_3}, \end{aligned} \tag{102}$$

where $\hat{R}_1$, $\hat{R}_2$, and $\hat{R}_3$ are the operator components of the rotation vector $\vec{R}$, defined in Fig. 1. Using Eq. (54), we write

$$\begin{aligned} H_r &= \frac{\hbar^2}{2\mathcal{I}} \left[\left(\vec{J} - \vec{j}\right)^2 - \left(\hat{J}_3 - \hat{j}_3\right)^2 \right] + \frac{\hbar^2}{2\mathcal{I}_3} \left(\hat{J}_3 - \hat{j}_3\right)^2 \\ &= \frac{\hbar^2}{2\mathcal{I}} \left[\left(\vec{J} - \vec{j}\right)^2 - (K - \Omega)^2 \right] + \frac{\hbar^2}{2\mathcal{I}_3} (K - \Omega)^2 \end{aligned} \tag{103}$$

where Ω is the projection of the intrinsic spin $\vec{j}$ on the 3-axis, and where we've replaced the operators $\hat{J}_3$ and $\hat{j}_3$ by their respective eigenvalues, K and Ω, in a basis of kets $|JMK\Omega\rangle$. Next, we write

$$\left(\vec{J} - \vec{j}\right)^2 = \hat{J}^2 - 2\hat{J}\hat{j} + \hat{j}^2, \tag{104}$$

where we've used the fact that the operators corresponding to the total angular momentum $\vec{J}$ and the intrinsic angular momentum $\vec{j}$ commute, because the rotational and intrinsic motion are independent. Using the ladder operators $\hat{J}_\pm \equiv \hat{J}_1 \pm \hat{J}_2$ and $\hat{j}_\pm \equiv \hat{j}_1 \pm \hat{j}_2$, we can expand the product of the operators $\hat{J}$ and $\hat{j}$ as

$$\begin{aligned} 2\hat{J}\hat{j} &= \hat{J}_+\hat{j}_- + \hat{J}_-\hat{j}_+ + 2\hat{J}_3\hat{j}_3 \\ &= \hat{J}_+\hat{j}_- + \hat{J}_-\hat{j}_+ + 2K\Omega \end{aligned} \tag{105}$$

where we've substituted the eigenvalues of $\hat{J}_3$ and $\hat{j}_3$ in the last step. Inserting Eqs. (104) and (105) in Eq. (103) we get

$$\begin{aligned} H_r &= \frac{\hbar^2}{2\mathcal{I}}\left[\hat{J}^2 - \hat{J}_+\hat{j}_- - \hat{J}_-\hat{j}_+ - 2K\Omega + \hat{j}^2 - (K-\Omega)^2\right] + \frac{\hbar^2}{2\mathcal{I}_3}(K-\Omega)^2 \\ &= \frac{\hbar^2}{2\mathcal{I}}\left[J(J+1) - K^2\right] + \frac{\hbar^2}{2\mathcal{I}_3}(K-\Omega)^2 - \frac{\hbar^2}{2\mathcal{I}}\left[\hat{J}_+\hat{j}_- + \hat{J}_-\hat{j}_+\right] + \frac{\hbar^2}{2\mathcal{I}}\left[\hat{j}^2 - \Omega^2\right] \end{aligned} \tag{106}$$

where we've substituted the eigenvalue $J(J+1)$ of the operator $\hat{J}^2$, and re-ordered the terms. The last two terms in Eq. (106) are associated with the particle-rotor coupling interaction and the intrinsic motion, respectively. We ignore the particle-rotor coupling, and absorb the intrinsic term into H_i in Eq. (53). the remaining terms in Eq. (106) are associated with the rotational energy

$$E_r(J,K) = \frac{\hbar^2}{2\mathcal{I}}\left[J(J+1) - K^2\right] + \frac{\hbar^2}{2\mathcal{I}_3}(K-\Omega)^2 . \tag{107}$$

In the limit of a perfect axial rotor, $\vec{R}$ is perpendicular to the 3-axis, and $\Omega \to K$. In that case, the second term in Eq. (107) vanishes, and we obtain the rotational energy for an axially-symmetric nucleus

$$E_r(J,K) = \frac{\hbar^2}{2\mathcal{I}_\perp}\left[J(J+1) - K^2\right], \tag{108}$$

where we've used $\mathcal{I}_\perp = \mathcal{I}_1 = \mathcal{I}_2 = \mathcal{I}$ for the moment of inertia about the axes perpendicular to the 3-axis. Conversely, if we observe a rotational level of spin J at energy E belonging to a band characterized by the quantum number K, then the band head is located at energy $E - E_r(J,K)$. Therefore, if we knew the state density $w(E,K)$ of intrinsic band heads with quantum number K, we could calculate the level density generated by all rotational bands producing levels with spin J in the neighborhood of energy E according to

$$\rho(E,J) = \frac{1}{2}\sum_{K=-J}^{J} w(E - E_r(J,K), K), \tag{109}$$

where the factor of 1/2 comes from the fact that the band members for an even-even axially symmetric nucleus characterized by the quantum number K are two-fold degenerate, as was shown in section III D 1 through symmetry considerations. In effect, the band members associated with $K \neq 0$ have spins $J = |K|, |K|+1, \ldots$. For simplicity, we ignore the special treatment of the case of $K = 0$ discussed in section III D 1.

To quantify the dependence of the state density in $w(E,K)$, we follow the derivation in [1], which is reminiscent of the discussion in section II. Referring to Fig. 1, we note that the projection Ω of the intrinsic spin on the 3-axis can be decomposed into contributions of the spin projections of unpaired valence nucleons, in other words

$$\Omega = \sum_i \Omega_i, \tag{110}$$

where the Ω_i represent the individual projections. If we assume that the Ω_i are independent, identically-distributed random variables (a form for that distribution is derived in [1]), we can then apply the central-limit theorem, as was done to obtain Eq. (9). Thus we write

$$w(E,\Omega) = w(E)\frac{1}{\sqrt{2\pi}\sigma_\|}e^{-\frac{\Omega^2}{2\sigma_\|^2}} \tag{111}$$

where $\rho_{intr}(E)$ designates the total intrinsic level density, and the parameter $\sigma_{\|}$, associated with the projections on the 3-axis, characterizes the width of the Gaussian distribution. In the limit of an axial rotor, $\Omega \to K$, and the intrinsic state density becomes

$$w(E,K) = w(E)\frac{1}{\sqrt{2\pi}\sigma_{\|}} e^{-\frac{K^2}{2\sigma_{\|}^2}}, \tag{112}$$

which is analogous to Eq. (9). The intrinsic state density can be taken as that of a Fermi gas, as in Eq. (52), or a more sophisticated form, discussed in section II B 5. In any case, the same exponential dependence on energy is obtained,

$$w(E) = f(E)e^{2\sqrt{aE}} \tag{113}$$

where $f(E)$ is a slowly-varying function of the energy (see the discussion in section II B 5). Using Eqs. (112) and (113) in Eq. (109), we get

$$\rho(E,J) = \frac{1}{2}\sum_{K=-J}^{J} f(E)e^{2\sqrt{a[E-E_r(J,K)]}} \frac{1}{\sqrt{2\pi}\sigma_{\|}} e^{-\frac{K^2}{2\sigma_{\|}^2}} \tag{114}$$

where we've assumed $E \gg E_r(J,K)$ and neglected the effect of the $-E_r(J,K)$ energy shift in the slowly-varying function $f(E)$. The energy dependence in the exponential can be expanded in a Taylor series for $E \gg E_r(J,K)$,

$$\begin{aligned} 2\sqrt{a[E-E_r(J,K)]} &\approx 2\sqrt{aE}\left[1 - \frac{1}{2E}E_r(J,K)\right] \\ &= 2\sqrt{aE} - \frac{1}{2\sigma_{\perp}^2}\left[J(J+1) - K^2\right], \end{aligned} \tag{115}$$

where we've defined the quantity

$$\sigma_{\perp}^2 \equiv \frac{1}{\hbar^2}\sqrt{\frac{E}{a}}\mathcal{I}_{\perp}. \tag{116}$$

With these simplifications, Eq. (114) becomes

$$\rho(E,J) = \frac{1}{2\sqrt{2\pi}\sigma_{\|}} f(E)e^{2\sqrt{aE}} e^{-\frac{J(J+1)}{2\sigma_{\perp}^2}} \sum_{K=-J}^{J} e^{-\left(\frac{1}{2\sigma_{\|}^2} - \frac{1}{2\sigma_{\perp}^2}\right)K^2}. \tag{117}$$

if we assume that the values of K in the sum are relatively small, that is if

$$\left(\frac{1}{2\sigma_{\|}^2} - \frac{1}{2\sigma_{\perp}^2}\right)K^2 \ll 1, \tag{118}$$

the sum over K yields $(2J+1)$, and Eq. (117) reduces to

$$\begin{aligned} \rho(E,J) &= \frac{2J+1}{2\sqrt{2\pi}\sigma_{\|}} f(E)e^{2\sqrt{aE}} e^{-\frac{J(J+1)}{2\sigma_{\perp}^2}} \\ &= \frac{2J+1}{2\sqrt{2\pi}\sigma_{\|}} w(E) e^{-\frac{J(J+1)}{2\sigma_{\perp}^2}}. \end{aligned} \tag{119}$$

E. Summary: collective enhancement factors

In this section we summarize the enhancement of the level density with respect to a spherical level density for the various symmetries discussed above. The level density for a spherical nucleus with state density $w(E)$ is given by Eq. (10),

$$\begin{aligned}\rho_{sph}(E,J) &= w(E) \times \frac{2J+1}{2\sqrt{2\pi}\sigma^3} \exp\left[-\frac{(J+1/2)^2}{2\sigma^2}\right] \\ &\approx w(E) \times \frac{2J+1}{2\sqrt{2\pi}\sigma^3} \exp\left[-\frac{J(J+1)}{2\sigma^2}\right], \end{aligned} \tag{120}$$

where we've used $(J+1/2)^2 \approx J(J+1)$. Then, according to Eq. (119), the enhancement factor for an axially-symmetric nucleus is

$$k_{ax}(E,J) \equiv \frac{\rho_{ax}(E,J)}{\rho_{sph}(E,J)} \approx \sigma_{\|}^2, \tag{121}$$

where we've assumed $\sigma \approx \sigma_\perp \approx \sigma_\|$.

Starting from an axially-symmetric nucleus, we can break the reflection symmetry with respect to a plane perpendicular to the 3-axis, which is implicit in the D_∞ symmetry group. As discussed in section III C, the breaking of this symmetry increases the level density by a factor of two. Thus, for a reflection-asymmetric nucleus

$$k_{ras}(E,J) = \frac{\rho_{ras}(E,J)}{\rho_{sph}(E,J)} = \frac{\rho_{ras}(E,J)}{\rho_{ax}(E,J)} \times \frac{\rho_{ax}(E,J)}{\rho_{sph}(E,J)} = 2\sigma_\|^2 \tag{122}$$

In the case of a nucleus with no rotational symmetry, the discussion in section III A leads us to expect an increase in the number of levels by a factor $(2J+1)$ for a given spin J. However, this does not provide us with a reasonable energy dependence of the enhancement factor. We can estimate the energy dependence by evaluating the stated density for a system with no symmetry, starting from Eq. (7b)

$$w_{ns}(E) = \sum_{J=0}^{\infty}(2J+1)\rho_{ns}(E,J). \tag{123}$$

where the subscript "ns" stands for "no symmetry". In the spirit of Eq. (109), we can relate the level density $\rho_{ns}(E,J)$ to the state density in a spherical nucleus

$$\rho_{ns}(E,J) = \sum_{K=-J}^{J} w_{sph}(E - E_r(J,K)), \tag{124}$$

where we do not have to correct for the two-fold degeneracy of the axially-symmetric case, as in Eq. (109). For $E \gg E_r(J,K)$, the energy-shifted state density can be approximated by a first-order Taylor expansion

$$w_{sph}(E - E_r(J,K)) \approx w_{sph}(E) - E_r(J,K)\frac{d}{dE}w_{sph}(E). \tag{125}$$

The derivative of the state density can be related to the nuclear temperature through the definition

$$\frac{1}{T} \equiv \frac{d}{dE} k \ln w_{sph}(E), \tag{126}$$

where k is the Boltzmann constant, and the quantity $k \ln w_{sph}(E)$ is the entropy. Using this definition of the temperature, Eq. (125) becomes

$$\begin{aligned} w_{sph}(E - E_r(J,K)) &\approx w_{sph}(E)\left[1 - \frac{E_r(J,K)}{kT}\right] \\ &\approx w_{sph}(E)e^{-\frac{E_r(J,K)}{kT}}, \end{aligned} \tag{127}$$

where we've assumed $E_r(J,K) \ll kT$ in the last step. Combining Eqs. (123), (124), (125), and (127), we get

$$w_{ns}(E) = w_{sph}(E)\sum_{J=0}^{\infty}\sum_{K=-J}^{J}(2J+1)e^{-\frac{E_r(J,K)}{kT}}. \tag{128}$$

In order to evaluate the sums, we go to the continuum limit. The sum over J carries over into an integral without complication. The projection K can be expressed in terms of the length J of the angular momentum, and the angle θ with respect to the 3-axis as $K \approx J\cos\theta$. An infinitesimal increment in K for a given J is given by $dK = Jd\cos\theta$. Then, if we assume $2J+1 \approx 2J$, we can make the substitution

$$\sum_{J=0}^{\infty}\sum_{K=-J}^{J}(2J+1) \to \int_0^{\infty} dJ \int_{-1}^{1} Jd\cos\theta\,\frac{1}{2\pi}\int_0^{2\pi} d\phi\,2J, \tag{129}$$

where we've added a dummy integration over the azimuthal angle ϕ. The integrals in Eq. (129) can be simplified into the suggestive form

$$\frac{1}{\pi}\int_0^{\infty} dJ J^2 \int_0^{\pi}\sin\theta d\theta \int_0^{2\pi} d\phi, \tag{130}$$

which we recognize as a volume integral in spherical coordinates. The same integral can also be written in Cartesian coordinates as

$$\frac{1}{\pi}\int_{-\infty}^{\infty} dJ_1 \int_{-\infty}^{\infty} dJ_2 \int_{-\infty}^{\infty} dJ_3. \tag{131}$$

We can expand $E_r(J,K)$ in Eq. (128) as [50]

$$E_r(J,K) = \frac{\hbar^2\hat{J}_1^2}{2\mathcal{I}_1} + \frac{\hbar^2\hat{J}_2^2}{2\mathcal{I}_2} + \frac{\hbar^2\hat{J}_3^2}{2\mathcal{I}_3}. \tag{132}$$

Combining Eqs. (128), (131), and (132), we write

$$w_{ns}(E) = w_{sph}(E)\frac{1}{\pi}\int_{-\infty}^{\infty} dJ_1 \int_{-\infty}^{\infty} dJ_2 \int_{-\infty}^{\infty} dJ_3\, e^{-\frac{1}{kT}\left[\frac{\hbar^2 J_1^2}{2\mathcal{I}_1} + \frac{\hbar^2 J_2^2}{2\mathcal{I}_2} + \frac{\hbar^2 J_3^2}{2\mathcal{I}_3}\right]} \tag{133}$$

If we treat J_1, J_2, and J_3 as variables, rather than operators, the three Gaussian integrals in Eq. (133) can be evaluated and the result is

$$w_{ns}(E) = w_{sph}(E)\sqrt{8\pi}\left[\frac{\mathcal{I}_1}{\hbar^2}\frac{\mathcal{I}_2}{\hbar^2}\frac{\mathcal{I}_3}{\hbar^2}(kT)^3\right]^{1/2} \tag{134}$$

IV. THE WASHING OUT OF COLLECTIVE ENHANCEMENTS

Nuclear shapes and the associated symmetries disappear with increasing excitation energy, as the nucleus assumes a spherical shape. In this section we will demonstrate this effect and provide a prescription for quantifying the washing out of collective enhancements with increasing excitation energy.

We begin by considering the relationship between nuclear shape and shell structure. The liquid-drop model (LDM) provides a convenient framework within which nuclear shape can be quantified. The important contributions to the LDM energy are the surface and Coulomb terms, which can be expanded in terms of the nuclear elongation (β) and axial asymmetry (γ) parameters [19, 31]

$$E_{LD} = V_{surf} + V_{Coul} = \frac{1}{2\pi} b_{surf} A^{2/3} \left[(1-x)\beta^2 - \frac{2}{21}\sqrt{\frac{5}{4\pi}}(1+2x)\beta^3 \cos 3\gamma \right] \tag{135}$$

where $b_{surf} \approx 17$ MeV, A is the mass of the nucleus, and x is its fissility, defined as

$$x \equiv \frac{Z^2/A}{(Z^2/A)_{crit}}, \tag{136}$$

and which is expressed relative to the critical value $(Z^2/A)_{crit} \approx 49$ MeV. For example, for ^{240}Pu in its axially-symmetric ground state ($\gamma = 0$), we have

$$E_{LD}\left(^{240}\text{Pu}\right) \approx 29.3\beta^2 - 15.3\beta^3 \text{ (MeV)} \tag{137}$$

The potential energy in Eq. (137) is plotted in Fig. 2 and displays a clear minimum for $\beta = 0$ (i.e., a spherical shape). But ^{240}Pu is known to have a deformed ground-state configuration with $\beta \sim 0.26$ (and $\gamma \neq 0$ as well) [32]. Non-spherical, static deformations arise purely because of nuclear shell effects. In fact, one could attempt to obtain the nuclear potential surface from microscopic arguments similar to the ones used to calculate level densities in section II B 1. In practice however, purely microscopic approaches do not accurately reproduce many features of deformed nuclei, such as fission-barrier properties. Therefore a "macroscopic-microscopic" treatment, wherein the best features of the LDM and microscopic calculations are combined, is usually preferred. There are various prescriptions for implementing this approach [33], but basically the microscopic calculation of the potential energy is split up into smooth and oscillating parts, and the oscillating part, which represents shell-structure effects, is recombined with the LDM prediction. The "Strutinsky-renormalization procedure" is a commonly-used prescription to carry out the separation of the potential energy into smooth and oscillating portions (see appendix E), but for pedagogic reasons, we will defer its discussion, and use the more familiar machinery of the partition-function method introduced in section II B 1.

A. A toy shell model

We will use the schematic model given in [34] to illustrate the separation of the nuclear energy into smooth and shell contributions in the partition-function formalism. In an extreme harmonic-oscillator model where the single-particle states in each shell are degenerate, with the same degeneracy Ω, and the shells are separated by the same spacing $\hbar\omega_{sh}$, the single-particle spectrum is given by

$$g(\epsilon) = \Omega \sum_{n=0}^{\infty} \delta(\epsilon - \epsilon_0 - n\hbar\omega_{sh}), \tag{138}$$

where ϵ_0 is the zero-point energy. For positive ϵ, the function $g(\epsilon)$ in Eq. (138) is periodic with period $2L = \hbar\omega_{sh}$. The function $g(\epsilon)$ can therefore be expanded in a Fourier series

$$g(\epsilon) = \sum_{k=-\infty}^{\infty} c_k e^{i\pi k\epsilon/L} \tag{139}$$

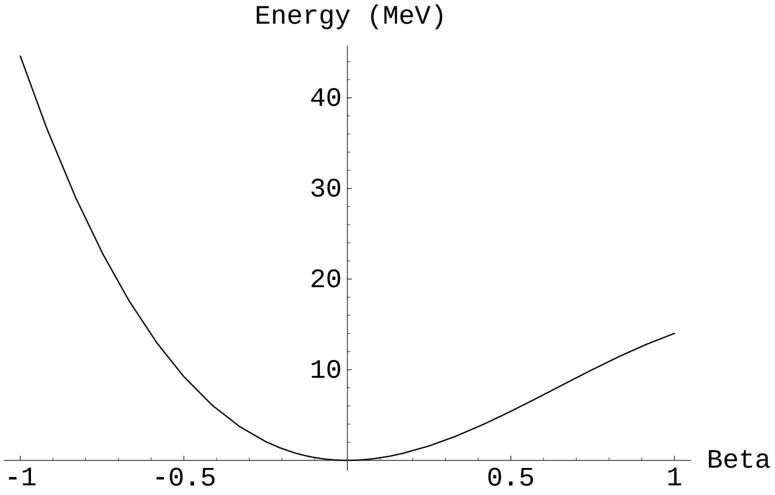

FIG. 2: Plot of the potential energy in Eq. (137) for ^{240}Pu.

with coefficients

$$\begin{aligned} c_k &\equiv \frac{1}{2L}\int_{-L}^{L} d\epsilon\, g(\epsilon) e^{-i\pi k\epsilon/L} \\ &= \frac{\Omega}{\hbar\omega_{sh}} e^{-\frac{2i\pi k\epsilon_0}{\hbar\omega_{sh}}} \end{aligned} \qquad (140)$$

Keeping only the first few terms in Eq. (139), we write

$$\begin{aligned} g(\epsilon) &\approx c_0 + c_1 e^{\frac{2i\pi\epsilon_0}{\hbar\omega_{sh}}} + c_{-1} e^{-\frac{2i\pi\epsilon_0}{\hbar\omega_{sh}}} \\ &= \frac{\Omega}{\hbar\omega_{sh}} + \frac{2\Omega}{\hbar\omega_{sh}} \cos\frac{2\pi(\epsilon-\epsilon_0)}{\hbar\omega_{sh}}. \end{aligned} \qquad (141)$$

For the purposes of the present discussion, we generalize Eq. (141) to the form

$$g(\epsilon) = g_0 + g_1 \cos\frac{2\pi(\epsilon-\epsilon_0)}{\hbar\omega_{sh}}, \qquad (142)$$

where g_0 represents a smooth spectrum, modulated by the cosine term with amplitude g_1. The more general form of Eq. (142), compared to Eq. (141), allows us to mimic the change in the shell structure with deformation, to some extent. If the shell structure is very pronounced, then we expect $g_1 \sim g_0$, if it is not then $g_1 \to 0$, and we revert back to a smooth, featureless single-particle spectrum. We will show that the energy obtained by placing particles in the single-particle spectrum of Eq. (142) can be divided into a smooth part and an oscillating part associated with the filling of the shells. It is tempting to think that the constant term in Eq. (142) will give rise to the smooth behavior in the energy, while the oscillatory term will single-handedly produce the shell effects; this is not entirely accurate. We will see that some care is required in separating the energy into smooth and shell contributions.

Starting from Eq. (142), we calculate the grand partition function given by Eq. (34). We will then be able to deduce the energy of the system from the constraint in Eq. (21a). We write

$$\begin{aligned}\ln Z(\alpha,\beta) &= g_0\int_0^\infty \ln\left(1+e^{\alpha-\beta\epsilon}\right)d\epsilon + g_1\int_0^\infty \cos\frac{2\pi(\epsilon-\epsilon_0)}{\hbar\omega_{sh}}\ln\left(1+e^{\alpha-\beta\epsilon}\right)d\epsilon \\ &\approx g_0\int_0^{\alpha/\beta}(\alpha-\beta\epsilon)\,d\epsilon + \frac{g_0\pi^2}{6\beta} \\ &\quad + g_1\int_0^\infty \cos\frac{2\pi(\epsilon-\epsilon_0)}{\hbar\omega_{sh}}\ln\left(1+e^{\alpha-\beta\epsilon}\right)d\epsilon \end{aligned} \tag{143}$$

where we've used the result in Eq. (42). In appendix C we show that, for large values of α and small values of ϵ_0, the oscillatory integral in Eq. (143) can be approximated by

$$\int_0^\infty \cos\frac{2\pi(\epsilon-\epsilon_0)}{\hbar\omega_{sh}}\ln\left(1+e^{\alpha-\beta\epsilon}\right)d\epsilon \approx -\frac{\hbar\omega_{sh}}{2}\frac{\cos\left[\frac{2\pi}{\hbar\omega_{sh}}\left(\frac{\alpha}{\beta}-\epsilon_0\right)\right]}{\sinh\left(\frac{2\pi^2}{\hbar\omega_{sh}\beta}\right)}. \tag{144}$$

Thus,

$$\ln Z(\alpha,\beta) \approx g_0\int_0^{\alpha/\beta}(\alpha-\beta\epsilon)\,d\epsilon + \frac{g_0\pi^2}{6\beta} - g_1\frac{\hbar\omega_{sh}}{2}\frac{\cos\left[\frac{2\pi}{\hbar\omega_{sh}}\left(\frac{\alpha}{\beta}-\epsilon_0\right)\right]}{\sinh\left(\frac{2\pi^2}{\hbar\omega_{sh}\beta}\right)}. \tag{145}$$

We apply the number constraint, Eq. (21a). The derivative of $\ln Z(\alpha,\beta)$ is relatively easy to calculate, and for a number A of particles we get

$$g_0\frac{\alpha}{\beta} + g_1\frac{\pi}{\beta}\frac{\sin\left[\frac{2\pi}{\hbar\omega_{sh}}\left(\frac{\alpha}{\beta}-\epsilon_0\right)\right]}{\sinh\left(\frac{2\pi^2}{\hbar\omega_{sh}\beta}\right)} = A, \tag{146}$$

where α and β are the saddle-point values of the Lagrange multipliers (we've dropped the "0" subscripts in Eq. (21) for convenience and assume that α and β are evaluated at the saddle point). The Fermi energy is always defined as $\epsilon_F \equiv \alpha/\beta$, and we introduce the variable

$$\tau \equiv \frac{2\pi^2}{\hbar\omega_{sh}\beta}. \tag{147}$$

Using these definitions, Eq. (146) can be re-written in the more compact form,

$$g_0\epsilon_F + g_1\frac{\hbar\omega_{sh}}{2\pi}\frac{\tau\sin\left[\frac{2\pi}{\hbar\omega_{sh}}(\epsilon_F-\epsilon_0)\right]}{\sinh\tau} = A. \tag{148}$$

On the other hand, if we ignore the oscillatory term in Eq. (142), we're back to the equidistant-level model, and we expect the energy of the system to vary smoothly and by small increments as each new particle is added. The Fermi energy in the case of $g_1 \to 0$ is given by Eq. (43a), or

$$\int_0^{\tilde{\epsilon}_F} d\epsilon\, g_0 = A \Rightarrow g_0\tilde{\epsilon}_F = A \tag{149}$$

where we've used the notation "$\tilde{\epsilon}_F$" to differentiate this Fermi energy from the one calculated for the full single-particle spectrum in Eq. (142). In fact, the Fermi energy ϵ_F, which appears in Eq. (146), can be thought of as consisting of a "smooth" contribution, namely $\tilde{\epsilon}_F$, and a contribution due to shell effects. The Fermi energy can be decomposed in this fashion by combining Eqs. (146) and (149),

$$\begin{aligned} g_0\tilde{\epsilon}_F &= A = g_0\epsilon_F + g_1\frac{\hbar\omega_{sh}}{2\pi}\frac{\tau\sin\left[\frac{2\pi}{\hbar\omega_{sh}}\left(\epsilon_F-\epsilon_0\right)\right]}{\sinh\tau} \\ \Rightarrow\ \epsilon_F &= \tilde{\epsilon}_F - \frac{g_1}{g_0}\frac{\hbar\omega_{sh}}{2\pi}\frac{\tau\sin\left[\frac{2\pi}{\hbar\omega_{sh}}\left(\epsilon_F-\epsilon_0\right)\right]}{\sinh\tau}. \end{aligned} \tag{150}$$

Note that ϵ_F still appears in the right-hand side of Eq. (150). However, it is important to note that ϵ_F appears only in the argument of the sine function, which is a bounded function. We will hide this dependence on ϵ_F by introducing the variable y, defined in [35] by

$$\epsilon_F = \epsilon_0 + \hbar\omega_{sh}\left(y-\frac{1}{2}\right), \tag{151}$$

and Eq. (150) reduces to the more compact form

$$\epsilon_F = \tilde{\epsilon}_F + \frac{g_1}{g_0}\frac{\hbar\omega_{sh}}{2\pi}\frac{\tau\sin\left(2\pi y\right)}{\sinh\tau}. \tag{152}$$

Eq. (152) is the reason why we must take some care in separating the smooth and shell contributions in the calculation of the energy of the system. We could not simply have used the single-particle spectrum in Eq. (142) with $g_0 \to 0$ and expected to extract the shell-dependent energy contribution directly, we must take into account the details of the Fermi energy.

We now return to the energy constraint in Eq. (21a) to evaluate the energy of the system. The derivative of $\ln Z(\alpha,\beta)$ with respect to the Lagrange multiplier β is a bit more cumbersome to calculate. Using the notation introduced above, we write the energy-constraint equation as

$$g_0\frac{\epsilon_F^2}{2} + g_0\frac{\pi^2}{6\beta^2} - g_1\frac{\hbar\omega_{sh}}{2\pi}\epsilon_F\tau\frac{\sin\left(2\pi y\right)}{\sinh\tau} - g_1\left(\frac{\hbar\omega_{sh}}{2\pi}\right)^2\tau^2\frac{\cosh\tau}{\sinh^2\tau}\cos\left(2\pi y\right) = E. \tag{153}$$

Replacing ϵ_F by its decomposition in Eq. (152) then yields

$$E = \underbrace{g_0\frac{\tilde{\epsilon}_F^2}{2} + g_0\frac{\pi^2}{6\beta^2}}_{\tilde{E}}\underbrace{-g_1\left(\frac{\hbar\omega_{sh}}{2\pi}\right)^2\frac{\tau^2}{\sinh^2\tau}\left[\cosh\tau\cos\left(2\pi y\right) + \frac{g_1}{2g_0}\sin^2\left(2\pi y\right)\right]}_{E_{sh}}, \tag{154}$$

where we've divided the energy E into a smooth contribution, that would be expected from a simple equidistant-level model of the single-particle spectrum (see Eq. (47)), and a leftover shell contribution.

In the limit of large temperatures, $T \to \infty \Rightarrow \beta \to 0 \Rightarrow \tau \to \infty$, the asymptotic form of the shell-energy contribution in Eq. (154) is

$$\begin{aligned} E_{sh}(\alpha,\beta) &\xrightarrow{T\to\infty} -2g_1\left(\frac{\hbar\omega_{sh}}{2\pi}\right)^2\tau^2 e^{-2\tau}\left[e^{\tau}\cos\left(2\pi y\right) + \frac{g_1}{g_0}\sin\left(2\pi y\right)\right] \\ &\xrightarrow{T\to\infty} 0. \end{aligned} \tag{155}$$

Note that the dependence of variable y on the temperature is irrelevant because the sine and cosine functions of y are bounded.

We can calculate other thermodynamic quantities of interest, such as the entropy defined in Eq. (48), using Eqs. (145), (148), and (153)

$$\begin{aligned} S &\equiv \ln Z(\alpha,\beta) - \alpha A + \beta E \\ &= \underbrace{g_0\frac{\pi^2}{3\beta}}_{\tilde{S}}\underbrace{-g_1\frac{\hbar\omega_{sh}}{2}\frac{\cos\left(2\pi y\right)}{\sinh\tau}\left(\tau\coth\tau - 1\right)}_{S_{sh}}, \end{aligned} \tag{156}$$

where we've again identified a smooth contribution $\tilde{S}$ (in analogy with Eq. (48)) associated with the constant part in the single-particle spectrum Eq. (142), and a leftover shell-dependent correction S_{sh}. In the limit of large temperatures, we have again

$$\begin{aligned} S_{sh} &\xrightarrow{T\to\infty} -g_1\hbar\omega_{sh}\cos(2\pi y)\,(\tau-1)e^{-\tau} \\ &\xrightarrow{T\to\infty} 0. \end{aligned} \tag{157}$$

The free energy, which can be thought of as a generalization of the potential energy for non-zero temperatures, can also be obtained from the energy in Eq. (154) and the entropy in Eq. (156)

$$\begin{aligned} F &\equiv E - \frac{S}{\beta} \\ &= \underbrace{g_0\frac{\tilde{\epsilon}_F}{2} - g_0\frac{\pi^2}{6\beta^2}}_{\tilde{F}} \underbrace{-g_1\left(\frac{\hbar\omega_{sh}}{2\pi}\right)^2\frac{\tau}{\sinh\tau}\left[\cos(2\pi y) + \frac{g_1}{2g_0}\frac{\tau\sin^2(2\pi y)}{\sinh\tau}\right]}_{F_{sh}}, \end{aligned} \tag{158}$$

where we've separated the smooth ($\tilde{F}$) and shell (F_{sh}) contributions in the usual manner. Once again, we take the limit of large temperatures,

$$\begin{aligned} F_{sh} &\xrightarrow{T\to\infty} -2g_1\left(\frac{\hbar\omega_{sh}}{2\pi}\right)^2\tau e^{-\tau}\cos(2\pi y) \\ &\xrightarrow{T\to\infty} 0. \end{aligned} \tag{159}$$

The nucleus will seek an equilibrium configuration that maximizes the entropy for a fixed energy or, equivalently, minimizes the free energy at fixed temperature. In either case, Eqs. (157) and (159) show that the contributions associated with shell effects disappears with increasing temperature (and therefore with increasing excitation energy). With increasing temperature, the nucleus therefore behaves more like a liquid drop, and its preferred equilibrium shape, dictated by Eq. (135), is spherical (i.e., $\beta = 0$).

B. Fundamental causes for the disappearance of shell structure

The disappearance of shell effects with increasing temperature observed in the toy model of section IV A is a general phenomenon, and not a consequence of the particular form of the single-particle spectrum. We could generalize the results above in a straightforward manner by including all the terms in the Fourier series in Eq. (141), but instead we will seek to understand what causes the disappearance of shell effects.

In order to understand what drives the washing out of the shell structure, we examine how the thermodynamic quantities calculated in section IV A are affected by the addition of a particle, causing a slight shift $\delta\epsilon_F$ in the Fermi energy. For a general single-particle spectrum $g(\epsilon)$, the energy of the system is obtained from Eq. (21a), omitting the "0" subscripts for convenience,

$$\begin{aligned} E &= -\frac{\partial}{\partial\beta}\int_0^\infty d\epsilon\, g(\epsilon)\ln\left[1+e^{\alpha-\beta\epsilon}\right] \\ &= \int_0^\infty d\epsilon\, g(\epsilon)\frac{e^{-\beta(\epsilon-\epsilon_F)}}{1+e^{-\beta(\epsilon-\epsilon_F)}}, \end{aligned} \tag{160}$$

where we've used the definition $\epsilon_F \equiv \alpha/\beta$ to eliminate α in Eq. (160). We recognize the Fermi-Dirac distribution function

$$f(\epsilon) \equiv \frac{e^{-\beta(\epsilon-\epsilon_F)}}{1+e^{-\beta(\epsilon-\epsilon_F)}}. \tag{161}$$

in Eq. (160). If we shift the Fermi energy by a small amount $\delta\epsilon_F$, the Fermi-Dirac distribution will also change by a small amount $\delta f(\epsilon)$ such that

$$\begin{aligned} f(\epsilon) + \delta f(\epsilon) &= \frac{e^{-\beta(\epsilon-\epsilon_F-\delta\epsilon_F)}}{1+e^{-\beta(\epsilon-\epsilon_F-\delta\epsilon_F)}} \\ \Rightarrow \ \delta f(\epsilon) &= \frac{e^{-\beta(\epsilon-\epsilon_F-\delta\epsilon_F)}}{1+e^{-\beta(\epsilon-\epsilon_F-\delta\epsilon_F)}} - \frac{e^{-\beta(\epsilon-\epsilon_F)}}{1+e^{-\beta(\epsilon-\epsilon_F)}} \\ \Rightarrow \ \delta f(\epsilon) &= \frac{\left(e^{\beta\delta\epsilon_F}-1\right) f(\epsilon)}{1+e^{\beta\delta\epsilon_F}e^{-\beta(\epsilon-\epsilon_F)}}. \end{aligned} \tag{162}$$

Thus, applying the shift $\epsilon_F \to \epsilon_F + \delta\epsilon_F$ to Eq. (160),

$$\begin{aligned} E + \delta E &= \int_0^\infty d\epsilon\, g(\epsilon)\, [f(\epsilon) + \delta f(\epsilon)] \\ \Rightarrow \ \delta E &= \int_0^\infty d\epsilon\, g(\epsilon) \delta f(\epsilon) \end{aligned} \tag{163}$$

Now we can study what happens to the incremental energy calculated in Eq. (163), in the limits of high and low temperatures. First, we assume that at any given temperature, we can always choose the increment in the Fermi energy to be small enough that $\beta\delta\epsilon_F \ll 1$. Then we can approximate Eq. (162) by

$$\delta f(\epsilon) \approx \beta\delta\epsilon_F \frac{f(\epsilon)}{1+e^{-\beta(\epsilon-\epsilon_F)}}. \tag{164}$$

In the low-temperature case ($T \to 0 \Rightarrow \beta \to \infty$), the Fermi-Dirac distribution function becomes a step function

$$f(\epsilon) \overset{\beta\to\infty}{\longrightarrow} \begin{cases} 1 & \epsilon < \epsilon_F \\ 1/2 & \epsilon = \epsilon_F \\ 0 & \epsilon > \epsilon_F \end{cases}. \tag{165}$$

Because of the asymptotic behavior of $f(\epsilon)$ in Eq. (165), the increment $\delta f(\epsilon)$, given by Eq. (164), vanishes when $\beta(\epsilon - \epsilon_F) \gg 1$. Furthermore, when $\beta(\epsilon - \epsilon_F) \ll -1$, the exponential in the denominator of Eq. (164) forces $\delta f(\epsilon)$ to vanish again. However, in the neighborhood of the Fermi energy, i.e. when $\beta(\epsilon - \epsilon_F) \approx 0$, $\delta f(\epsilon)$ is finite and has approximate value

$$\delta f(\epsilon_F) \approx \frac{1}{4}\beta\delta\epsilon_F. \tag{166}$$

This, in turn, implies that in the limit of low temperatures, the bulk of the contribution to the integral in Eq. (163) comes from energies ϵ in an interval centered about the Fermi energy and of width comparable to the temperature.

Conversely, at high temperatures ($T \to \infty \Rightarrow \beta \to 0$), $\delta f(\epsilon)$ in Eq. (164) assumes the constant value in Eq. (166) at all energies ϵ. In that case, the integral in Eq. (163) is an average over all energies, and not just those energies near the Fermi level.

Therefore, if there are shell structures in $g(\epsilon)$ on an energy scale which is small compared to the temperature, they will be erased by the integral over all energies in Eq. (163), and the increment δE in energy will depend on the increment in the Fermi energy (and therefore on the addition of particles) in a smooth way. If, on the other hand, the shell structure is large compared to the temperature, the integral in Eq. (163) will be sensitive to this shell structure, and δE could jump suddenly with the addition of particles. Thus, the appearance or washing-out of shell effects is tied to the temperature of the system. These conclusions can be extended to other thermodynamic variables, such as the entropy and the free energy by following the same procedure.

C. Coda: a measure of the disappearance of shell effects

In section IV A and IV B we investigated the causes for the disappearance of shell effects with increasing nuclear temperature and the subsequent return to a spherical nuclear shape. In this section, we provide a practical way of quantifying this effect. The formalism derived here is taken principally from [36], and gives the probability that a nucleus at a given temperature will have a particular shape.

In the present approach, we treat the collective (e.g., rotational) and internal degrees of freedom as thermodynamic systems that can exchange energy, but nothing else (i.e., the microcanonical regime). We assume the density of states corresponding to the internal degrees of freedom can be calculated (e.g. by the technique described in section II B 1). The collective states will be counted using a semi-classical approach [37] which we review presently.

Fig. 3a) shows the path in phase space taken by a system undergoing periodic motion in one dimension (x is the position, and $p(x)$ is its conjugate momentum). This motion can be quantized using the Bohr-Sommerfeld rule [38]

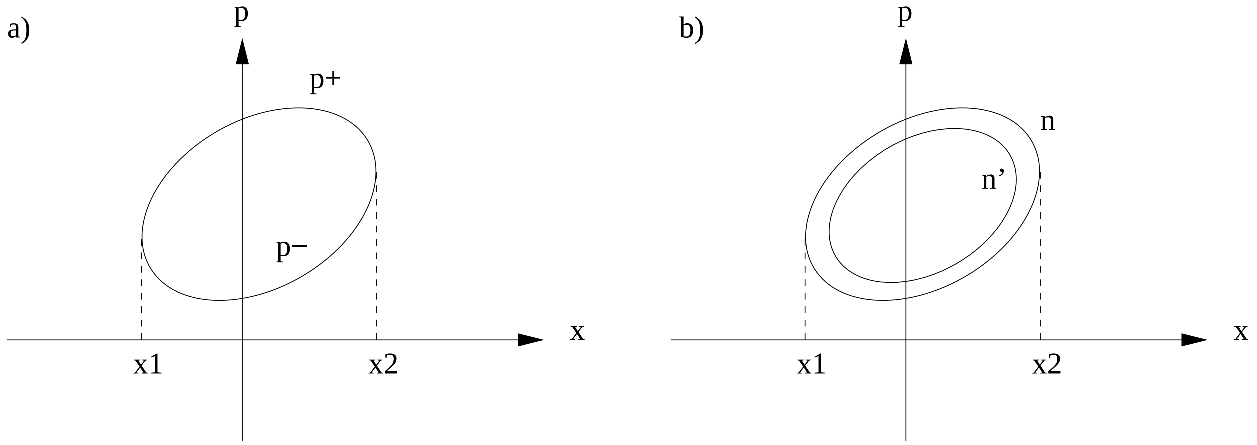

FIG. 3: Illustration of one-dimensional motion depicted in (two-dimensional) phase space. Panel a) shows the function $p_+(x)$ evaluated from position x_1 to x_2, and the function $p_-(x)$, evaluated from x_2 back to x_1. Panel b) shows two different quantizations, labeled by quantum numbers n and n', according the the Bohr-Sommerfeld rule.

$$\oint p(x)dx = nh, \tag{167}$$

where n is an integer, h is Planck's constant, and the integral can be written in terms of the upper ($p_+(x)$) and lower ($p_-(x)$) portions of the two-valued function $p(x)$, in other words

$$nh = \int_{x_1}^{x_2} p_+(x)dx + \int_{x_2}^{x_1} p_-(x)dx = \int_{x_1}^{x_2} p_+(x)dx - \int_{x_1}^{x_2} p_-(x)dx. \tag{168}$$

This integral is simply the area enclosed by the contour in Fig. 3a).

When quantized according to Eq. (167), each contour in phase space corresponds to a state, labeled by the quantum number n. Fig. 3b) shows the contours for two states labeled by n and $n' < n$. There are $n - n'$ contours (and therefore states) between the ones drawn in the figure. The difference $n - n'$ is just the area of the shell between the contours, divided by Planck's constant

$$\Delta n = n - n' = \frac{1}{h} \oint \Delta p \, dx. \tag{169}$$

The most elementary element of area in phase space is therefore

$$\frac{dp \, dx}{h}, \tag{170}$$

and must be integrated along the trajectory in phase space to yield the incremental number of states.

We now describe the coupling between collective and internal degrees of freedom in the microcanonical picture. The collective motion is characterized by the deformation ϵ (we ignore other collective variables for simplicity), and its conjugate momentum p. The energy of the collective motion is

$$E_{coll} = \frac{p^2}{2m}, \tag{171}$$

where m is the inertial mass associated with the collective motion. The incremental number of collective states is given by Eq. (170), with the deformation variable ϵ playing the role of the position x. The probability of finding the collective and internal systems in a particular set of states for a given total energy is proportional to the density of internal states (w_{int}) times the density of collective states (w_{coll}). The excitation energy E_x of the nucleus will distribute itself into internal (E_{int}) and collective (E_{coll}, given by Eq. (171)) contributions,

$$E_x = E_{int} + E_{coll}. \tag{172}$$

The probability of finding the nucleus with deformation between ϵ and $\epsilon + \delta\epsilon$ and momentum between p and $p + \delta p$ is then given by

$$P(\epsilon, p)\delta\epsilon\delta p = \frac{1}{\mathcal{N}} w_{int}(E_{int}) \times \delta N_{coll}(E_{coll}), \tag{173}$$

where $\mathcal{N}$ is a constant chosen to normalize the probability to 1. We will not need to calculate $\mathcal{N}$ because we will be interested in relative probabilities only. The incremental number of collective states $\delta N_{coll}(E_{coll})$ is given by Eq. (170). Since we are only interested in the deformation parameter, we can integrate out the momentum dependence to find the probability

$$P(\epsilon)\delta\epsilon = \frac{\delta\epsilon}{\mathcal{N}h} \int w_{int}\left(E_x - \frac{p^2}{2m}\right) dp. \tag{174}$$

The integral in Eq. (174) must be carried out over all possible values of p. However, by construction, there are no internal states for $E_{int} < 0$, therefore the integral can be restricted to the range $-\sqrt{2mE_x} \leq p \leq \sqrt{2mE_x}$. It is safe to assume that the density of internal states, w_{int}, increases very rapidly with the internal energy, therefore most of the contribution to the integral in Eq. (174) will come from a region near $p = 0$, where the argument of w_{int} is maximized. Thus we can: 1) approximate the integral by extending the integration limits to $\pm\infty$, and 2) expand the integrand in a Taylor series about $p = 0$. We begin by writing Eq. (174) in a more useful form,

$$P(\epsilon)\delta\epsilon \approx \frac{\delta\epsilon}{\mathcal{N}h} \int_{-\infty}^{\infty} e^{\ln\left[w_{int}\left(E_x - p^2/(2m)\right)\right]} dp. \tag{175}$$

It will be more effective to expand the logarithm in Eq. (175) in a Taylor series about $p = 0$, rather than the function w_{int} itself, because the exponential will force a faster convergence of the integral. The approximation procedure so far shares some features in common with the saddle-point approximation, discussed in appendix A, however, this is not a saddle-point approximation. Although we will be expanding the argument of the exponential in Eq. (175) in a Taylor series, we will not be looking for contribution from a "critical point" where the argument is extremized.

The Taylor series we want is

$$\begin{aligned} \ln\left[w_{int}\left(E_x - \frac{p^2}{2m}\right)\right] &= \ln\left[w_{int}\left(E_x\right)\right] - \left(\frac{\partial}{\partial x} \ln\left[w_{int}(x)\right]\right)\Bigg|_{x=E_x} \frac{p^2}{2m} \\ &+ \frac{1}{2}\left(\frac{\partial^2}{\partial x^2} \ln\left[w_{int}(x)\right]\right)\Bigg|_{x=E_x} \left(-\frac{p^2}{2m}\right)^2 + \cdots \end{aligned} \tag{176}$$

Since most of the contribution to the integral in Eq. (175) will come from small values of p, we can truncate the Taylor series at the term of order p^2. Then, Eq. (175) reduces to the evaluation of a Gaussian integral

$$P(\epsilon)\delta\epsilon \approx \frac{\delta\epsilon}{\mathcal{N}h} w_{int}\left(E_x\right) \int_{-\infty}^{\infty} dp \exp\left[-\left(\frac{\partial}{\partial x} \ln\left[w_{int}(x)\right]\right)\Bigg|_{x=E_x} \frac{p^2}{2m}\right]. \tag{177}$$

We examine the derivative term in the exponent more closely,

$$\frac{\partial}{\partial x}\ln\left[w_{int}(x)\right]\bigg|_{x=E_x} = \frac{1}{w_{int}(E_x)}\frac{\partial}{\partial x}w_{int}(x)\bigg|_{x=E_x}. \tag{178}$$

The dummy variable x in Eq. (178) plays the role of an energy. We can use the partition-function relation in Eq. (13) to evaluate the derivative in Eq. (178),

$$\frac{\partial}{\partial x}\ln\left[w_{int}(x)\right]\bigg|_{x=E_x} = \frac{1}{w_{int}(E_x)}\beta w_{int}(E_x) = \beta \equiv \frac{1}{kT}, \tag{179}$$

where we've introduced the definition of β in terms of the temperature T and the Boltzmann constant k. Now the integral in Eq. (177) takes the form

$$\begin{aligned} P(\epsilon)\delta\epsilon &\approx \frac{\delta\epsilon}{\mathcal{N}h}w_{int}\left(E_x\right)\int_{-\infty}^{\infty}dp\,\exp\left[-\frac{p^2}{2mkT}\right] \\ &= \frac{\sqrt{2\pi mkT}}{\mathcal{N}h}w_{int}\left(E_x\right)\delta\epsilon. \end{aligned} \tag{180}$$

The dependence of the right-hand-side of Eq. (180) on deformation is introduced through the total energy E_{tot}, defined as

$$E_{tot} = E_x + V(\epsilon), \tag{181}$$

where $V(\epsilon)$ is the deformation-dependent potential energy. Then, Eq. (180) becomes

$$P(\epsilon)\delta\epsilon \approx \frac{\sqrt{2\pi mkT}}{\mathcal{N}h}w_{int}\left(E_{tot} - V(\epsilon)\right)\delta\epsilon. \tag{182}$$

The result in Eq. (182) has been derived assuming a single collective variable, the deformation parameter ϵ. The Generalization of this formalism to an arbitrary number of collective variables is discussed in [39].

For a given total energy E_{tot}, the probability in Eq. (182) varies as a function of deformation. In fact, according to Eq. (182), we expect that the most likely deformation of the nucleus will be found where $V(\epsilon)$ is smallest (and therefore the excitation energy highest). As was discussed in sections IV and IV B, the potential $V(\epsilon)$, corrected for shell effects, tends toward the liquid-drop limit with increasing temperature. As $T \to \infty$, we expect that the lowest value of $V(\epsilon)$ will occur at $\epsilon = 0$, and therefore this is where $P(\epsilon)\delta\epsilon$ in Eq. (182) will reach its highest value.

Using the probability in Eq. (182) as a weight it may be possible to calculate the number of levels at each temperature, averaged over all possible deformations. The resulting level density would display the expected washing out of collective enhancements with increasing excitation energy. To the best of our knowledge, the use of Eq. (182) to estimate this behavior has been hinted at (see the discussion at the end of [2]), but never carried out in the literature.

V. ACKNOWLEDGMENTS

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APPENDIX A: THE SADDLE-POINT APPROXIMATION

We wish to approximate integrals of the form of Eq. (13). In general, these are integrals in the complex plane that can be cast into the form

$$\int_{z_1}^{z_2} dz\, e^{f(z)}, \tag{A1}$$

where $f(z)$ is an analytic function (i.e., differentiable in the complex plane), at least in some region of the complex plane. By a corollary of Cauchy's theorem, it is always possible to distort the integration path in Eq. (A1), provided the endpoints z_1 and z_2 remain the same and the path does not go through any singularities [40]. In particular, we will show that it is always possible to choose the integration path such that most of the contribution to the integral comes from a small region around a special point, z_0. The integral can then be approximated by the evaluation of the integrand at z_0, with a normalization factor taking into account the behavior of $f(z)$ in the immediate neighborhood of z_0.

The optimal integration path then is one where the real part of $f(z)$, $\Re\{f(z)\}$, reaches a maximum, positive value at a point z_0, while the imaginary part, $\Im\{f(z)\}$, remains constant along the path and near z_0 [51]. Maximizing the real part of $f(z)$ ensures that the integrand in Eq. (A1) will give its largest contribution near z_0, while keeping the imaginary part constant prevents oscillations in the integrand which might cancel out the contribution from $\Re\{f(z)\}$. What may be surprising, is that the requirement that $f(z)$ be analytic guarantees that it is possible to simultaneously maximize $\Re\{f(z)\}$ while keeping $\Im\{f(z)\}$ constant.

To illustrate this property of analytic functions, we consider the particular case of the function

$$f(z) \equiv z^2 = \underbrace{x^2 - y^2}_{u(x,y)} + \underbrace{2xy}_{v(x,y)}\, i, \tag{A2}$$

where we've defined the real and imaginary parts of the function, $u(x, y)$ and $v(x, y)$, respectively. This is an analytic function and its derivative in the complex plane is $f'(z) = 2z$. The real and imaginary parts of $f(z)$ are not independent, in fact if we calculate tangent vectors $\nabla u(x, y)$ and $\nabla v(x, y)$ to their respective contours,

$$\begin{aligned} \nabla u(x,y) &= (2x, -2y) \\ \nabla v(x,y) &= (2y, 2x), \end{aligned} \tag{A3}$$

we find that these contours are everywhere orthogonal to each other:

$$[\nabla u(x, y)] \cdot [\nabla v(x, y)] = 2xy - 2xy = 0. \tag{A4}$$

Eq. (A4) shows that it is possible to move in the direction of increasing $\Re\left\{z^2\right\} \equiv u(x, y)$, while moving along contours of constant $\Im\left\{z^2\right\} \equiv v(x, y)$ (i.e., in the direction of $\nabla v(x, y)$). This can be seen more clearly in Fig. 4, where the real and imaginary contours of $f(z) = z^2$ are plotted.

The result we have obtained for the particular function $f(z) = z^2$ can be generalized to any analytic function. The fact that $f(z)$ is differentiable implies that the value of the derivative $f'(z)$ at a point z is unique, which requires that the Cauchy-Riemann equations are satisfied

$$\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y} \\ \frac{\partial v}{\partial x} &= -\frac{\partial u}{\partial y}. \end{aligned} \tag{A5}$$

As in the case of the z^2 function, we see that the contour lines of u and v are orthogonal to each other everywhere,

$$\begin{aligned} [\nabla u(x, y)] \cdot [\nabla v(x, y)] &= \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\frac{\partial v}{\partial y} \\ &= -\frac{\partial u}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial u}{\partial y}\frac{\partial u}{\partial x} \\ &= 0. \end{aligned} \tag{A6}$$

Now we seek the critical point z_0 where $\Re\{f(z)\}$ is maximized along the integration path. By the Cauchy-Riemann equations, Eq. (A5), we see that

$$\begin{aligned} &\frac{\partial u}{\partial x} = 0 \;\Rightarrow\; \frac{\partial v}{\partial y} = 0 \\ &\frac{\partial u}{\partial y} = 0 \;\Rightarrow\; \frac{\partial v}{\partial x} = 0, \end{aligned} \tag{A7}$$

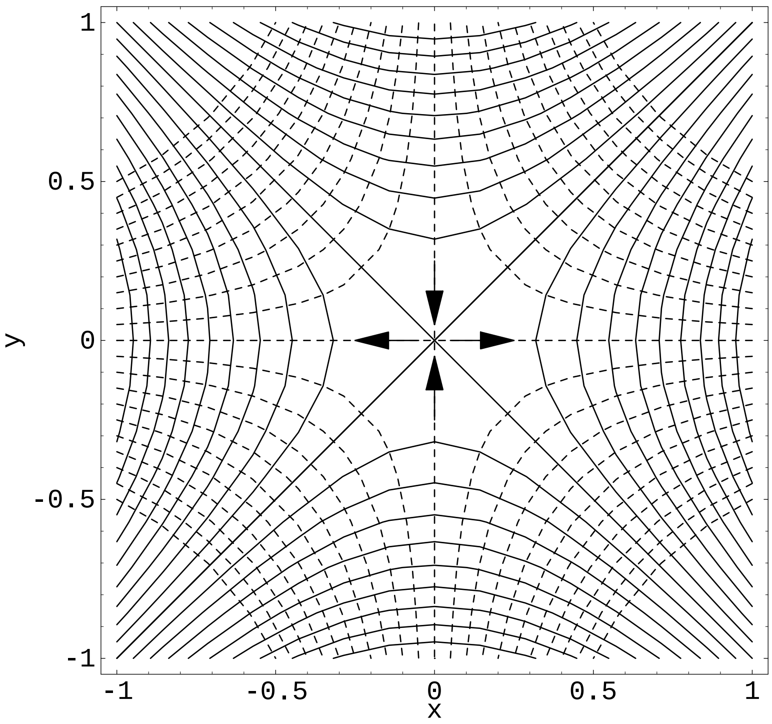

FIG. 4: Contour lines for $u(x,y)$ (solid lines) and $v(x,y)$ (dotted lines) for the z^2 function (see Eq. (A2)). The arrows indicate directions along which $u(x,y) = \Re\left\{z^2\right\}$ increases while $v(x,y) = \Im\left\{z^2\right\}$ remains constant.

and extremizing the real part of $f(z)$ also requires that the imaginary part be an extremum. The critical point z_0 must therefore satisfy

$$f'(z_0) = 0. \tag{A8}$$

However, $f(z_0)$ is neither a maximum nor a minimum, but a saddle point [52]. This follows from the Cauchy-Riemann equations because

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 v}{\partial x \partial y} = \frac{\partial}{\partial y}\left(-\frac{\partial u}{\partial y}\right) = -\frac{\partial^2 u}{\partial y^2}, \tag{A9}$$

and similarly for the imaginary part,

$$\frac{\partial^2 v}{\partial x^2} = -\frac{\partial^2 u}{\partial x \partial y} = -\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial y}\right) = -\frac{\partial^2 v}{\partial y^2}, \tag{A10}$$

and what is a maximum (minimum) with respect to x is therefore a minimum (maximum) with respect to y.

Near the critical point z_0, the function $f(z)$ can be expanded in a Taylor series

$$f(z) = f(z_0) + \frac{1}{2}f''(z_0)(z - z_0)^2 + \cdots \tag{A11}$$

If we assume $f''(z_0) \neq 0$, we can discard the higher-order terms in Eq. (A11), so that

$$f(z) \approx f(z_0) + \frac{1}{2}f''(z_0)(z - z_0)^2. \tag{A12}$$

The contour lines of the real and imaginary parts of Eq. (A12) look like the ones for the z^2 function in Fig. 4, except that they are displaced by z_0, and rotated by the phase of $f''(z_0)$. Writing the magnitude and phase explicitly,

$$\begin{aligned} f''(z_0) &\equiv \rho_0 e^{i\delta_0} \\ z - z_0 &\equiv t\, e^{i\phi} \end{aligned} \tag{A13}$$

where $\rho_0 \geq 0$ and $t \geq 0$. Eq. (A12) becomes

$$f(z) \approx f(z_0) + \frac{1}{2}\rho_0 t^2 e^{i(\delta_0 + 2\phi)} \tag{A14}$$

from which,

$$\begin{aligned} \Re\{f(z)\} &\approx \Re\{f(z_0)\} + \frac{1}{2}\rho_0 t^2 \cos(\delta_0 + 2\phi) \\ \Im\{f(z)\} &\approx \Im\{f(z_0)\} + \frac{1}{2}\rho_0 t^2 \sin(\delta_0 + 2\phi). \end{aligned} \tag{A15}$$

Remember that we want to approach z_0 along a path where $\Im\{f(z)\}$ is constant, and $\Re\{f(z)\}$ increases to a maximum value. By inspection of Eq. (A15), we see that this can be accomplished if we choose the phase ϕ such that

$$\delta_0 + 2\phi = \pi. \tag{A16}$$

The integral in Eq. (A1) can now be evaluated along an optimal path which satisfies the condition in Eq. (A16) near z_0. Conversely, far from z_0, we can adjust the path such that the imaginary part of $f(z)$ varies as rapidly as possible and the real part is small or even negative, so that the contribution to the integral from the portions of the path far from z_0 is made small. Thus most of the contribution to the integral will come from the path C_0 in some neighborhood of z_0. Using Eqs. (A14) and (A16), we write

$$\int_{z_1}^{z_2} dz\, e^{f(z)} \approx e^{f(z_0)} \int_{C_0} e^{-\frac{1}{2}\rho_0 t^2} e^{i\phi} dt. \tag{A17}$$

As we move away from z_0, t increases and the integrand in Eq. (A17) becomes small. Therefore, we can further approximate the integral with respect to t by evaluating from $-\infty$ to ∞,

$$\begin{aligned} \int_{z_1}^{z_2} dz\, e^{f(z)} &\approx e^{f(z_0)} e^{i\phi} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\rho_0 t^2} dt \\ &= e^{f(z_0)} e^{i\phi} \sqrt{\frac{2\pi}{\rho_0}}. \end{aligned} \tag{A18}$$

We can manipulate Eq. (A18) to get rid of the explicit dependence on the phase ϕ,

$$\begin{aligned} \int_{z_1}^{z_2} dz\, e^{f(z)} &\approx e^{f(z_0)} e^{i\phi} \sqrt{\frac{2\pi e^{i\delta_0}}{\rho_0 e^{i\delta_0}}} \\ &= e^{f(z_0)} \sqrt{\frac{2\pi e^{i(\delta_0 + 2\phi)}}{f''(z_0)}} \\ &= i\, e^{f(z_0)} \sqrt{\frac{2\pi}{f''(z_0)}}, \end{aligned} \tag{A19}$$

where we've used Eq. (A16) in the last step. The explicit appearance of the factor i in Eq. (A19) should not be cause for concern; if the integration path lies entirely along the real axis, then $f''(z_0)$ will be a negative number (because $f(z_0)$ is a maximum), and the i factor in front will serve to keep the integral in Eq. (A19) real.

As an illustration, we apply the saddle-point approximation in Eq. (A19) to the state density calculation in Eq. (13) by making the following substitutions in Eq. (A19)

$$\begin{aligned} f(\beta) &\equiv \ln Z(\beta) + \beta E \\ f''(\beta) &= \frac{\partial^2}{\partial\beta^2} \ln Z(\beta). \end{aligned} \tag{A20}$$

Then,

$$\begin{aligned} w(E) &= \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} Z(\beta) e^{\beta E} d\beta \\ &= \frac{1}{2\pi i} \times i \; e^{\ln Z(\beta)+\beta E} \sqrt{\frac{2\pi}{\frac{\partial^2}{\partial\beta^2} \ln Z(\beta)}} \Bigg|_{\beta_0} \\ &= \frac{e^{\ln Z(\beta)+\beta E}}{\sqrt{2\pi} \left[\frac{\partial^2}{\partial\beta^2} \ln Z(\beta)\right]^{1/2}} \Bigg|_{\beta_0} , \end{aligned} \tag{A21}$$

where the critical point β_0 is determined by the extremizing condition

$$f'(\beta_0) = 0 \tag{A22}$$

Eqs. (A21) and (A22) correspond directly to Eqs. (15) and (14), respectively.

APPENDIX B: CALCULATION OF THE MATRIX ELEMENT $D^J_{K'K}(0, \pi, 0)$

An intuitive approach to evaluate $D^J_{K'K}(0, \pi, 0)$ is suggested in [41]. In this appendix we present this approach in detail for the case where J is even. The matrix element $D^J_{K'K}(0, \pi, 0)$ implies a rotation through angle π of the body-fixed coordinate frame, about the 2-axis. We consider first the rotation of the fully aligned state with projection $K = J$. Microscopically, this state can be formed by $2J$ spin-1/2 nucleons aligned in a parallel configuration. (This is a conceptual construct, therefore there is no rotational angular momentum vector $\vec{R}$ to contend with, as in Eq. (54).) We can deduce the effect of the rotation on the angular-momentum J state from its effect on the individual spin-1/2 states.

The rotation operator $R_2^{(1/2)}(\pi)$ for spin-1/2 systems can be expressed in terms of Pauli spin matrix s_y,

$$R_2^{(1/2)}(\pi) = e^{-\pi i s_y} = e^{-\pi i \sigma_y/2}, \tag{B1}$$

where

$$\sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{B2}$$

It is easy to verify that

$$\sigma_y^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I, \tag{B3}$$

where I is the identity matrix. We can simplify Eq. (B1) using Eq. (B3)

$$\begin{aligned} e^{-\pi i \sigma_y/2} &= 1 - \frac{\pi i}{2}\sigma_y + \frac{1}{2!}\left(\frac{-\pi i}{2}\right)^2 \sigma_y^2 + \frac{1}{3!}\left(\frac{-\pi i}{2}\right)^3 \sigma_y^3 + \cdots \\ &= \left[1 + \frac{1}{2!}\left(\frac{-\pi i}{2}\right)^2 + \cdots\right] + \left[-\frac{\pi i}{2} + \frac{1}{3!}\left(\frac{-\pi i}{2}\right)^3 + \cdots\right]\sigma_y \\ &= \cos\frac{\pi}{2} - i\sigma_y \sin\frac{\pi}{2} \\ &= -i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \end{aligned} \tag{B4}$$

The rotation of a single spin-1/2 state with positive alignment along the 3-axis is performed by applying the matrix operator in Eq. (B4) to the spin-up vector, in matrix notation

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{B5}$$

Thus, the effect is to flip a spin-up state into a spin-down state, and the corresponding phase factor is +1. We can transform each of the $2J$ spin-1/2 states that add up to J in the same way. Then the rotation of the fully-aligned state with angular momentum J yields

$$R_2(\pi)\,|J, K = J\rangle = |J, K = -J\rangle \tag{B6}$$

The rotation of states other than $|J, K = J\rangle$ can be calculated by constructing the other states from the fully aligned one. We present a brief review of how the appropriate states are constructed, to draw attention to the subtleties of working in the body-fixed coordinate system. Recall the commutation relations (Eq. (63)) in the body-fixed frame

$$[\hat{J}_1, \hat{J}_2] = -i\hat{J}_3, [\hat{J}_2, \hat{J}_3] = -i\hat{J}_1, [\hat{J}_3, \hat{J}_1] = -i\hat{J}_2, \tag{B7}$$

where we've set $\hbar = 1$ for convenience. Notice the minus signs in Eq. (B7), which was explained in the context of Eq. (63). We form the usual ladder operators

$$\begin{aligned} \hat{J}_+ &\equiv \hat{J}_1 + i\hat{J}_2 \\ \hat{J}_- &\equiv \hat{J}_1 - i\hat{J}_2, \end{aligned} \tag{B8}$$

and calculate their commutation relations with $\hat{J}_3$

$$\begin{aligned} \left[\hat{J}_3, \hat{J}_+\right] &= [\hat{J}_3, \hat{J}_1] + i[\hat{J}_3, \hat{J}_2] = -\hat{J}_+ \\ \left[\hat{J}_3, \hat{J}_-\right] &= [\hat{J}_3, \hat{J}_1] - i[\hat{J}_3, \hat{J}_2] = \hat{J}_-. \end{aligned} \tag{B9}$$

The matrix element of $\hat{J}_+$ between generic states $|J, K\rangle$ and $|J, K'\rangle$ can be evaluated using Eq. (B9)

$$\begin{aligned} \langle J, K'|\hat{J}_+|J, K\rangle &= \langle J, K'| - [\hat{J}_3, \hat{J}_+]|J, K\rangle \\ &= \langle J, K'|\hat{J}_+\hat{J}_3 - \hat{J}_3\hat{J}_+|J, K\rangle \\ &= (K - K')\,\langle J, K'|\hat{J}_+|J, K\rangle\,. \end{aligned} \tag{B10}$$

Then, assuming that $\langle J, K'|J_+|J, K\rangle \neq 0$, we must have

$$K - K' = 1. \tag{B11}$$

Stated differently, this means

$$\hat{J}_+ \left|J, K\right\rangle = c_+(K) \left|J, K-1\right\rangle , \tag{B12}$$

where $c_+(K)$ is a constant to be determined. Notice that, because of the commutation relations in Eq. (B7), the operator $\hat{J}_+$ reduces the projection K by one unit. We can calculate the constant $c_+(K)$ using Eq. (B12) and the orthogonality of the $\left|J, K-1\right\rangle$ kets

$$\begin{aligned} |c_+(K)|^2 &= \langle J, K-1|c_+^*(K)c_+(K)|J, K-1\rangle \\ &= \langle J, K|\hat{J}_+^\dagger \hat{J}_+|J, K\rangle \\ &= \langle J, K|\hat{J}_- \hat{J}_+|J, K\rangle , \end{aligned} \tag{B13}$$

where we've used Eq. (B8) in the last step. However,

$$\begin{aligned} \hat{J}_- \hat{J}_+ \left|J, K\right\rangle &= (\hat{J}_1 - i\hat{J}_2)(\hat{J}_1 + i\hat{J}_2) \left|J, K\right\rangle \\ &= (\hat{J}_1^2 + \hat{J}_2^2 + i[\hat{J}_1, \hat{J}_2]) \left|J, K\right\rangle \\ &= (\hat{J}^2 - \hat{J}_3^2 + \hat{J}_3) \left|J, K\right\rangle \\ &= [J(J+1) - K(K-1)] \left|J, K\right\rangle \end{aligned} \tag{B14}$$

where we've written the eigenvalues of the operators $\hat{J}$ and $\hat{J}_3$ in the last step. Combining Eqs. (B13) and (B14), we deduce the value of $c_+(K)$, up to a phase factor and write Eq. (B12) as

$$\hat{J}_+ \left|J, K\right\rangle = \underbrace{\sqrt{J(J+1) - K(K-1)}}_{c_+(K)} \left|J, K-1\right\rangle . \tag{B15}$$

A similar derivation gives the result for the coefficient $c_-(K)$ associated with the application of the $\hat{J}_-$ operator

$$\hat{J}_- \left|J, K\right\rangle = \underbrace{\sqrt{J(J+1) - K(K+1)}}_{c_-(K)} \left|J, K+1\right\rangle . \tag{B16}$$

We now return to the problem at hand of calculating the rotation of a state that is not fully aligned. consider the state $\left|J, K = J-1\right\rangle$ for example. We can use a ladder operator to build this state from the fully aligned state. Using Eq. (B15), we write

$$\begin{aligned} \left|J, K = J-1\right\rangle &= \frac{1}{c_+(K=J)} \hat{J}_+ \left|J, K = J\right\rangle \\ &= \frac{1}{\sqrt{2J}} \hat{J}_+ \left|J, K\right\rangle . \end{aligned} \tag{B17}$$

Next, we rotate this state,

$$R_2(\pi) \left|J, K = J-1\right\rangle = \frac{1}{c_+(K=J)} R_2(\pi) \hat{J}_+ \left|J, K = J\right\rangle . \tag{B18}$$

Before we can proceed further, we need to know how to commute operators $R_2(\pi) = e^{-\pi i \hat{J}_2}$ and $\hat{J}_+ = \hat{J}_1 + i\hat{J}_2$. The result

$$e^{-\pi i \hat{J}_2} \hat{J}_2 = \hat{J}_2 e^{-\pi i \hat{J}_2} \tag{B19}$$

can be readily checked by expanding the exponential as a series in $\hat{J}_2$. The commutation relation with $\hat{J}_1$ is not as easily obtained. We must first prove an important operator identity, the Campbell-Baker-Hausdorff expansion formula which, given operators A and B, and a constant λ states that

$$e^{\lambda B} A e^{-\lambda B} = A + \lambda[B, A] + \frac{\lambda^2}{2!}[B, [B, A]] + \cdots \tag{B20}$$

Eq. (B20) is not especially difficult to prove. We define the function

$$F(\lambda) \equiv e^{\lambda B} A e^{-\lambda B}, \tag{B21}$$

and, assuming $F(\lambda)$ is differentiable, we calculate

$$\begin{aligned} F'(\lambda) &= B e^{\lambda B} A e^{-\lambda B} - e^{\lambda B} A B e^{-\lambda B} \\ &= B e^{\lambda B} A e^{-\lambda B} - e^{\lambda B} A e^{-\lambda B} B \\ &= [B, F(\lambda)]. \end{aligned} \tag{B22}$$

If $F(\lambda)$ is infinitely differentiable, we can use Eq. (B22) to calculate higher-order derivatives recursively. For example

$$F''(\lambda) = [B, F'(\lambda)] = [B, [B, F(\lambda)]], \tag{B23}$$

and so on. Thus we can expand $F(\lambda)$ in a Taylor series about $\lambda = 0$

$$F(\lambda) = e^{\lambda B} A e^{-\lambda B} = A + \lambda[B, A] + \frac{\lambda^2}{2!}[B, [B, A]] + \cdots, \tag{B24}$$

which proves Eq. (B20). We can use this result to calculate the commutation of $e^{-\pi i \hat{J}_2}$ and $\hat{J}_1$ by setting $A = \hat{J}_1$, $B = \hat{J}_2$, and $\lambda = -\pi i$ in Eq. (B20). Then,

$$e^{-\pi i \hat{J}_2} \hat{J}_1 e^{\pi i \hat{J}_2} = \hat{J}_1 - \pi i[\hat{J}_2, \hat{J}_1] + \frac{(-\pi i)^2}{2!}\left[\hat{J}_2, [\hat{J}_2, \hat{J}_1]\right] + \cdots \tag{B25}$$

We use Eq. (B7) to calculate the needed commutators

$$\begin{aligned} [\hat{J}_2, \hat{J}_1] &= i\hat{J}_3 \\ \left[\hat{J}_2, [\hat{J}_2, \hat{J}_1]\right] &= [\hat{J}_2, i\hat{J}_3] = i[\hat{J}_2, \hat{J}_3] = \hat{J}_1 \\ \left[\hat{J}_2, \left[\hat{J}_2, [\hat{J}_2, \hat{J}_1]\right]\right] &= [\hat{J}_2, \hat{J}_1] = i\hat{J}_3 \\ &\vdots \ , \end{aligned} \tag{B26}$$

and we can see that the values of the commutators cycle between $i\hat{J}_3$ and $\hat{J}_1$. Therefore,

$$\begin{aligned} e^{-\pi i \hat{J}_2} \hat{J}_1 e^{\pi i \hat{J}_2} &= \left[1 + \frac{(-\pi i)^2}{2!} + \cdots\right] \hat{J}_1 + i\left[(-\pi i) + \frac{(-\pi i)^3}{3!} + \cdots\right] \hat{J}_3 \\ &= (\cos\pi)\, \hat{J}_1 + (\sin\pi)\, \hat{J}_3 \\ &= -\hat{J}_1, \end{aligned} \tag{B27}$$

from which

$$e^{-\pi i \hat{J}_2} \hat{J}_1 = -\hat{J}_1 e^{-\pi i \hat{J}_2}. \tag{B28}$$

Combining this result with Eq. (B19) and the definition in Eq. (B8), we conclude that

$$e^{-\pi i\hat{J}_2}\hat{J}_+ = e^{-\pi i\hat{J}_2}(\hat{J}_1 + i\hat{J}_2) = (-\hat{J}_1 + i\hat{J}_2)e^{-\pi i\hat{J}_2} = -\hat{J}_- e^{-\pi i\hat{J}_2}. \tag{B29}$$

Eq. (B18) can now be simplified using Eqs. (B6), (B16) and (B29)

$$\begin{aligned}
R_2(\pi)\left|J, K = J-1\right\rangle &= \frac{1}{c_+(K=J)}R_2(\pi)\hat{J}_+\left|J, K = J\right\rangle \\
&= -\frac{1}{c_+(K=J)}\hat{J}_- e^{-\pi i\hat{J}_2}\left|J, K = J\right\rangle \\
&= -\frac{1}{c_+(K=J)}\hat{J}_-\left|J, K = -J\right\rangle \\
&= -\frac{c_-(K=-J)}{c_+(K=J)}\left|J, K = -J+1\right\rangle \\
&= -\left|J, K = -(J-1)\right\rangle .
\end{aligned} \tag{B30}$$

The effect of the rotation by π about the 2-axis on the state with $K = J - 1$ is therefore: (i) a change in the sign of the projection on the 3-axis, and (ii) the appearance of a phase factor of -1. Next, We apply the rotation to the $K = J - 2$ state,

$$\begin{aligned}
R_2(\pi)\left|J, K = J-2\right\rangle &= R_2(\pi)\frac{1}{c_+(K=J-1)}\hat{J}_+\left|J, K = J-1\right\rangle \\
&= -\frac{1}{c_+(K=J-1)}\hat{J}_- R_2(\pi)\left|J, K = J-1\right\rangle \\
&= \frac{1}{c_+(K=J-1)}\hat{J}_-\left|J, K = -(J-1)\right\rangle \\
&= \frac{c_-(K=-(J-1))}{c_+(K=J-1)}\left|J, K = -(J-1)+1\right\rangle \\
&= \left|J, K = -(J-2)\right\rangle .
\end{aligned} \tag{B31}$$

Thus the trend is that the phase changes sign for every reduction of the projection by one unit. To rotate a state with arbitrary projection K, the lowering operator J_+ must be apply $J - K$ times to the fully aligned state. Therefore we have

$$R_2(\pi)\left|J, K\right\rangle = (-1)^{J-K}\left|J, -K\right\rangle . \tag{B32}$$

Returning to the definition of the Wigner D functions in Eq. (65), we write

$$\begin{aligned}
D^J_{K'K}(0,\pi,0) &= \langle JK'|R_2(\pi)|JK\rangle \\
&= (-1)^{J-K}\delta_{K',-K}
\end{aligned} \tag{B33}$$

APPENDIX C: EVALUATION OF THE GRAND PARTITION FUNCTION FOR AN OSCILLATORY SPECTRUM

In this appendix we calculate the integral in Eq. (144). The result is given in [35] with few details. Since the integration involves several subtle tricks and approximations, we derive it in detail here.

The integral we wish to evaluate is

$$I_0 \equiv \int_0^\infty \cos\frac{2\pi(\epsilon - \epsilon_0)}{\hbar\omega_{sh}} \ln\left(1 + e^{\alpha - \beta\epsilon}\right) d\epsilon. \tag{C1}$$

For convenience, we replace the cosine by a complex exponential and define

$$\begin{aligned} I_1 &\equiv \int_0^\infty e^{\frac{2\pi i(\epsilon-\epsilon_0)}{\hbar\omega_{sh}}} \ln\left(1+e^{\alpha-\beta\epsilon}\right) d\epsilon \\ &= e^{-ia} \underbrace{\int_0^\infty e^{\frac{2\pi i\epsilon}{\hbar\omega_{sh}}} \ln\left(1+e^{\alpha-\beta\epsilon}\right) d\epsilon}_{I_2}, \end{aligned} \tag{C2}$$

where we've defined $a \equiv 2\pi\epsilon_0/(\hbar\omega_{sh})$ for compactness of notation. Integral I_2 defined in Eq. (C2) can be reduced if we evaluate it by parts,

$$\begin{aligned} I_2 &\equiv \int_0^\infty \underbrace{d\epsilon\, e^{\frac{2\pi i\epsilon}{\hbar\omega_{sh}}}}_{\equiv dv} \underbrace{\ln\left(1+e^{\alpha-\beta\epsilon}\right)}_{\equiv u} \\ &= \frac{\hbar\omega_{sh}}{2\pi i}\, e^{\frac{2\pi i\epsilon}{\hbar\omega_{sh}}} \ln\left(1+e^{\alpha-\beta\epsilon}\right)\Big|_0^\infty + \frac{\hbar\omega_{sh}}{2\pi i}\beta \int_0^\infty d\epsilon\, e^{\frac{2\pi i\epsilon}{\hbar\omega_{sh}}} \frac{e^{\alpha-\beta\epsilon}}{1+e^{\alpha-\beta\epsilon}} \\ &= -\frac{\hbar\omega_{sh}}{2\pi i}\ln\left(1+e^{\alpha}\right) + \frac{\hbar\omega_{sh}}{2\pi i}\beta e^{\alpha} \underbrace{\int_0^\infty d\epsilon\, \frac{e^{\left(-\beta+\frac{2\pi i}{\hbar\omega_{sh}}\right)\epsilon}}{1+e^{\alpha-\beta\epsilon}}}_{I_3} \end{aligned} \tag{C3}$$

Making the substitution $x \equiv -\alpha + \beta\epsilon$, the integral I_3 in Eq. (C3) can be re-written as

$$I_3 = \frac{1}{\beta} e^{\frac{\alpha}{\beta}\left(-\beta+\frac{2\pi i}{\hbar\omega_{sh}}\right)} \underbrace{\int_{-\alpha}^\infty dx\, \frac{e^{\left(-1+\frac{2\pi i}{\hbar\omega_{sh}\beta}\right)x}}{1+e^{-x}}}_{I_4} \tag{C4}$$

So far, we have made no approximations, but integral I_4, defined in Eq. (C4) cannot be evaluated in closed form for arbitrary values of α and $2\pi/(\hbar\omega_{sh}\beta)$. However, the integral I_4 can be further simplified if we assume $\alpha \gg 1$. In that case we can write the approximate value

$$I_4 \approx \int_{-\infty}^\infty dx\, \frac{e^{(-1+ib)x}}{1+e^{-x}}, \tag{C5}$$

where we've define $b \equiv 2\pi/(\hbar\omega_{sh}\beta)$ for more compact notation. The integral in Eq. (C5) can be evaluated by calculating the contour integral

$$\oint dz\, \frac{e^{(-1+ib)z}}{1+e^{-z}}, \tag{C6}$$

along the semicircular contour defined in Fig. 5, in the limit $R \to \infty$. The integrand in Eq. (C6) has poles along the imaginary axis at $z_k = (2k+1)\pi i$, where $k = 0, \pm 1, \pm 2, \cdots$. The residues at those points are

$$\begin{aligned} a_{-1}^{(k)} &= \lim_{z\to z_k} \frac{e^{(-1+ib)z}}{1+e^{-z}} \\ &= -e^{-(2k+1)b\pi}. \end{aligned} \tag{C7}$$

Only those poles with $k \geq 0$ fall within the contour of Fig. 5, thus

$$\begin{aligned} \oint dz\, \frac{e^{(-1+ib)z}}{1+e^{-z}} &= 2\pi i \sum_{k=0}^\infty -e^{-(2k+1)b\pi} \\ &= -2\pi i e^{-b\pi} \sum_{k=0}^\infty e^{-2kb\pi} \\ &= \frac{-2\pi i e^{-b\pi}}{1-e^{-2b\pi}}. \end{aligned} \tag{C8}$$

The integral along contour C_2 in Fig. 5 vanishes as $R \to \infty$, and the integral along C_1 becomes identical to Eq. (C5). Therefore,

$$I_4 \approx \frac{-2\pi i e^{-b\pi}}{1 - e^{-2b\pi}} = \frac{-\pi i}{\sinh(\pi b)} \tag{C9}$$

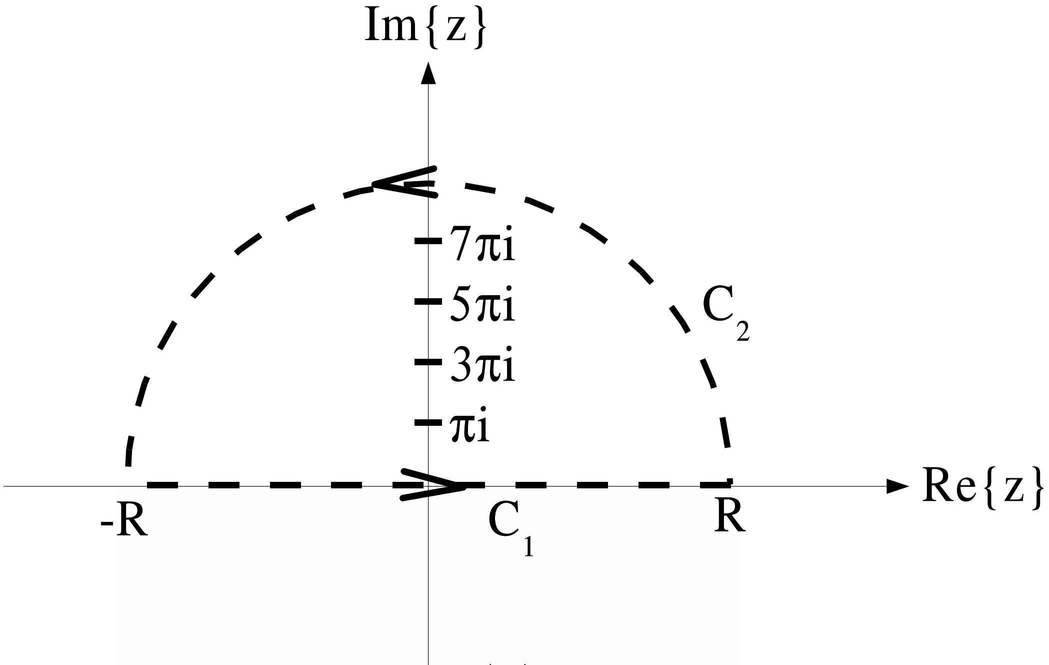

FIG. 5: Semicircular contour used to evaluate the integral in Eq. (C6), drawn with dashes. The closed contour is subdivided into segments C_1 and C_2 to aid in the discussion.

Finally, we return to Eq. (C1), and using the result in Eq. (C9), we write

$$\begin{aligned} I_0 &= \Re\{I_1\} \\ &\approx \frac{\sin a}{b\beta} \ln\left(1 + e^{\alpha}\right) - \frac{\pi}{b\beta} \frac{\cos\left(\alpha b - a\right)}{\sinh(\pi b)}. \end{aligned} \tag{C10}$$

In the limit where $\alpha \gg 1$, we can simplify the first term in Eq. (C10)

$$\frac{\sin a}{b\beta} \ln\left(1 + e^{\alpha}\right) \approx \frac{\alpha}{\beta}\frac{\sin a}{b} = \epsilon_F \frac{\sin a}{b}, \tag{C11}$$

where $\epsilon_F \equiv \alpha/\beta$ is the Fermi energy. If we further assume that ϵ_0 is very small, we can take the limit $a \to 0$, and the term in Eq. (C11) becomes negligible. Then Eq. (C10) becomes

$$I_0 \approx -\frac{\pi}{b\beta}\frac{\cos\left(\alpha b - a\right)}{\sinh(\pi b)}, \tag{C12}$$

which is the form used in Eq. (144).

APPENDIX D: LEVEL-DENSITY CALCULATION WITH PAIRING

In this section, we obtain the grand partition function and deduce the state density when we take into account the pairing correlations between nucleons. A similar derivation can be found in [39]. In order to introduce pairing between nucleons, we are led to single out one quantum number among the others: the projection of angular momentum on an arbitrary z axis. The pairing interaction will favor the coupling of nucleons into time-reversed orbitals (and therefore with opposite signs of the angular-momentum projection). In a spherical nucleus, the fermion creation operator for a state with spin j and angular momentum m is related to the creation operator of the time-reversed orbital $\overline{m}$ by [42]

$$a^{\dagger}_{j,\overline{m}} \equiv (-1)^{j+m} a^{\dagger}_{j,-m} \tag{D1}$$

where we've used the Biedenharn-Rose phase convention. In a deformed nucleus with axial symmetry, the projection on the symmetry axis is still a good quantum number, and the states with a given projection ν, or the time-reversed $\overline{\nu}$ can be expanded in a spherical basis

$$\begin{aligned} a^{\dagger}_{\nu} &= \sum_{j}\sum_{m=-j}^{j} c^{\nu}_{j,m} a^{\dagger}_{j,m} \\ a^{\dagger}_{\overline{\nu}} &= \sum_{j}\sum_{m=-j}^{j} c^{\nu}_{j,m} a^{\dagger}_{j,\overline{m}} \end{aligned} \tag{D2}$$

where the $c^{\nu}_{j,m}$ are expansion coefficients. The Hamiltonian for a deformed system with the simplest for of the pairing interaction is usually written [42]

$$H = \underbrace{\sum_{\nu} \epsilon_{\nu} a^{\dagger}_{\nu} a_{\nu}}_{H_0} \underbrace{-G \sum_{\mu,\nu>0} a^{\dagger}_{\mu} a^{\dagger}_{\overline{\mu}} a_{\overline{\nu}} a_{\nu}}_{H_{int}} \tag{D3}$$

where G is the (positive) interaction strength. The index in the first sum, labeled by H_0, in Eq. (D3) runs over all possible values of the angular-momentum projection ν. In the second sum, labeled by H_{int}, the indices μ and ν only run over half the allowed values, the contribution from the other half, corresponding to the time-reversed orbitals, is included explicitly in the creation and destruction operators. In effect H_0 represents the energy in an independent-particle model, while H_{int} introduces the residual coupling interaction. From the creation and destruction operators, it can be seen that the residual pairing interaction, $\propto (a^{\dagger}_{\mu} a^{\dagger}_{\overline{\mu}})(a_{\overline{\nu}} a_{\nu})$, scatters a pair of nucleons in time-reversed orbitals $(\nu, \overline{\nu})$ into another pair of time-reversed orbitals $(\mu, \overline{\mu})$.

In section II B 1, we were able to calculate the partition function and, ultimately, the state density starting from a Hamiltonian of the same form as H_0 in Eq. (D3) (compare with Eq. (18) assuming $n_{\nu} \equiv a^{\dagger}_{\nu} a_{\nu}$), but the interaction term H_{int} presents a different challenge. The solution to this and other problems involving the pairing interaction is to transform the Hamiltonian in Eq. (D3) into an independent-particle form like that of H_0. This is the essence of the Bardeen-Cooper-Schrieffer (BCS) theory [43].

The first step is to reduce the four-operator products in H_{int} in Eq. (D3) into two-operator products. This task can be accomplished through the mean-field approximation. We can always write

$$\begin{aligned} a_\mu^\dagger a_{\overline{\mu}}^\dagger &= \langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle + (a_\mu^\dagger a_{\overline{\mu}}^\dagger - \langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle) \\ a_{\overline{\nu}} a_\nu &= \langle a_{\overline{\nu}} a_\nu\rangle + (a_{\overline{\nu}} a_\nu - \langle a_{\overline{\nu}} a_\nu\rangle), \end{aligned} \tag{D4}$$

where we've separated each two-operator product in H_{int} into a mean part and a fluctuation about that mean. Note that, under normal circumstances, we would expect to have $\langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle = \langle a_{\overline{\nu}} a_\nu\rangle = 0$ because the bilinear operator products $a_\mu^\dagger a_{\overline{\mu}}^\dagger$ and $a_{\overline{\nu}} a_\nu$ change the number of particles in the system; the fact that we do not assume the mean values are identically zero is an indication that the means are calculated with respect to states without a well-defined number of particles. Next we use the mean-field approximation to calculate the four-operator product

$$\begin{aligned} a_\mu^\dagger a_{\overline{\mu}}^\dagger a_{\overline{\nu}} a_\nu &= \left[\langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle + (a_\mu^\dagger a_{\overline{\mu}}^\dagger - \langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle)\right] \times \left[\langle a_{\overline{\nu}} a_\nu\rangle + (a_{\overline{\nu}} a_\nu - \langle a_{\overline{\nu}} a_\nu\rangle)\right] \\ &\approx \langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle\, a_{\overline{\nu}} a_\nu + \langle a_{\overline{\nu}} a_\nu\rangle\, a_\mu^\dagger a_{\overline{\mu}}^\dagger - \langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle \langle a_{\overline{\nu}} a_\nu\rangle\,, \end{aligned} \tag{D5}$$

where we've neglected the product of the fluctuations as a 2nd order effect. We define the parameter Δ as

$$\Delta \equiv G \sum_{\nu>0} \langle a_{\overline{\nu}} a_\nu\rangle\,, \tag{D6}$$

and its complex conjugate is

$$\Delta^* \equiv G \sum_{\mu>0} \langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle\,. \tag{D7}$$

Using Eqs. (D5), (D6), and (D7) we can simplify H_{int} in Eq. (D3) to the bilinear form

$$\begin{aligned} H_{int} &= -G \sum_{\nu,\mu>0} \left(\langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle\, a_{\overline{\nu}} a_\nu + \langle a_{\overline{\nu}} a_\nu\rangle\, a_\mu^\dagger a_{\overline{\mu}}^\dagger - \langle a_\mu^\dagger a_{\overline{\mu}}^\dagger\rangle \langle a_{\overline{\nu}} a_\nu\rangle\right) \\ &= -\Delta^* \sum_{\nu>0} a_{\overline{\nu}} a_\nu - \Delta \sum_{\mu>0} a_\mu^\dagger a_{\overline{\mu}}^\dagger + \frac{|\Delta|^2}{G} \end{aligned} \tag{D8}$$

We have obtained a simpler form of H_{int} in Eq. (D8), but in applying the mean-field approximation, we've had to give up the concept of a well-defined particle number. We can still require conservation of the average number of particles by introducing a Lagrange multiplier for the Hamiltonian of Eq. (D3)

$$H \to H - \lambda \underbrace{\sum_\nu a_\nu^\dagger a_\nu}_{\hat{\mathcal{N}}}, \tag{D9}$$

where λ is the Lagrange multiplier, and $\hat{\mathcal{N}}$ is the standard number operator. Now the Hamiltonian in Eq. (D3) can be re-written in the mean-field approximation and with the modification of Eq. (D9) as

$$\begin{aligned} H &= \sum_\nu (\epsilon_\nu - \lambda)\, a_\nu^\dagger a_\nu - \Delta^* \sum_{\nu>0} a_{\overline{\nu}} a_\nu - \Delta \sum_{\mu>0} a_\mu^\dagger a_{\overline{\mu}}^\dagger + \frac{|\Delta|^2}{G} \\ &= \sum_{\nu>0} (\epsilon_\nu - \lambda)\, a_\nu^\dagger a_\nu + \sum_{\nu>0} (\epsilon_\nu - \lambda)\, a_{\overline{\nu}}^\dagger a_{\overline{\nu}} - \Delta^* \sum_{\nu>0} a_{\overline{\nu}} a_\nu - \Delta \sum_{\mu>0} a_\mu^\dagger a_{\overline{\mu}}^\dagger + \frac{|\Delta|^2}{G}, \end{aligned} \tag{D10}$$

where we've implicitly assumed $\epsilon_\nu = \epsilon_{\overline{\nu}}$. The next step is to diagonalize the Hamiltonian in Eq. (D10).

Diagonalizing the Hamiltonian in Eq. (D10) amounts to transforming the particle operators a into a new set of "quasi-particle" operators b, such that the only remaining operator products are of the diagonal form $b_\nu^\dagger b_\nu$ or $b_{\overline{\nu}}^\dagger b_{\overline{\nu}}$. This is accomplished by the Bogoliubov transformation

$$\begin{aligned} a_\nu &= u_\nu b_\nu + v_\nu b_{\overline{\nu}}^\dagger \\ a_{\overline{\nu}}^\dagger &= u_\nu b_{\overline{\nu}}^\dagger - v_\nu b_\nu . \end{aligned} \tag{D11}$$

Without loss of generality, we have assumed that the coefficients u_ν and v_ν in Eq. (D11) are real numbers, because any complex phase factor can simply be absorbed into the definition of the b operators. The transformation in Eq. (D11) is made unitary by imposing the condition

$$u_\nu^2 + v_\nu^2 = 1 \tag{D12}$$

It can be shown using Eqs. (D11) that imposing the condition in Eq. (D12) means that the quasi-particle operators will satisfy the same fermion anticommutation relations as the particle operators, i.e.

$$\begin{aligned} \{b_\nu^\dagger, b_{\nu'}\} &= \delta_{\nu,\nu'} \\ \left\{b_\nu^\dagger, b_{\nu'}^\dagger\right\} &= \{b_\nu, b_{\nu'}\} = 0 \end{aligned} \tag{D13}$$

For clarity, we apply the Bogoliubov transformation to the separate parts of the Hamiltonian in Eq. (D10)

$$\begin{aligned} H_0 &= \sum_{\nu>0} (\epsilon_\nu - \lambda)\, a_\nu^\dagger a_\nu + \sum_{\nu>0} (\epsilon_\nu - \lambda)\, a_{\overline{\nu}}^\dagger a_{\overline{\nu}} \\ &= \sum_{\nu>0} (\epsilon_\nu - \lambda) \left(u_\nu^2 - v_\nu^2\right) \left(b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}}\right) + 2\sum_{\nu>0} (\epsilon_\nu - \lambda)\, v_\nu^2 \\ &\quad +2\sum_{\nu>0} (\epsilon_\nu - \lambda)\, u_\nu v_\nu \left(b_\nu^\dagger b_{\overline{\nu}}^\dagger + b_{\overline{\nu}} b_\nu\right), \end{aligned} \tag{D14}$$

where we used the anticommutation relations in Eq. (D13) to order the operator products, and

$$\begin{aligned} H_{int} &= -\Delta^* \sum_{\nu>0} a_{\overline{\nu}} a_\nu - \Delta \sum_{\mu>0} a_\mu^\dagger a_{\overline{\mu}}^\dagger + \frac{|\Delta|^2}{G} \\ &= (\Delta + \Delta^*) \sum_{\nu>0} u_\nu v_\nu \left(b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}}\right) - (\Delta + \Delta^*) \sum_{\nu>0} u_\nu v_\nu + \frac{|\Delta|^2}{G} \\ &\quad - \sum_{\nu>0} \left(\Delta u_\nu^2 - \Delta^* v_\nu^2\right) b_\nu^\dagger b_{\overline{\nu}}^\dagger - \sum_{\nu>0} \left(\Delta^* u_\nu^2 - \Delta v_\nu^2\right) b_{\overline{\nu}} b_\nu . \end{aligned} \tag{D15}$$

Combining Eqs. (D14) and (D15), the total Hamiltonian is

$$\begin{aligned} H &= \sum_{\nu>0} \left[(\epsilon_\nu - \lambda)\left(u_\nu^2 - v_\nu^2\right) + (\Delta + \Delta^*)\, u_\nu v_\nu\right] \left(b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}}\right) \\ &\quad +2\sum_{\nu>0} (\epsilon_\nu - \lambda)\, v_\nu^2 - (\Delta + \Delta^*) \sum_{\nu>0} u_\nu v_\nu + \frac{|\Delta|^2}{G} \\ &\quad +\sum_{\nu>0} \underbrace{\left[2(\epsilon_\nu - \lambda)\, u_\nu v_\nu - \left(\Delta u_\nu^2 - \Delta^* v_\nu^2\right)\right]}_{w_\nu} b_\nu^\dagger b_{\overline{\nu}}^\dagger \\ &\quad +\sum_{\nu>0} \underbrace{\left[2(\epsilon_\nu - \lambda)\, u_\nu v_\nu - \left(\Delta^* u_\nu^2 - \Delta v_\nu^2\right)\right]}_{w_\nu^*} b_{\overline{\nu}} b_\nu , \end{aligned} \tag{D16}$$

where the coefficients multiplying the bilinear products $b_\nu^\dagger b_{\overline{\nu}}^\dagger$ and $b_{\overline{\nu}} b_\nu$ have been labeled as w_ν and its complex conjugate w_ν^*, respectively. These bilinear operator products must be eliminated in order to cast the Hamiltonian into a diagonal form, therefore we choose the coefficients u_ν and v_ν such that

$$w_\nu \equiv 2\left(\epsilon_\nu - \lambda\right) u_\nu v_\nu - \left(\Delta u_\nu^2 - \Delta^* v_\nu^2\right) = 0, \tag{D17}$$

which also implies $w_\nu^* = 0$. Eq. (D17) can be separated into its real and imaginary parts

$$2\left(\epsilon_\nu - \lambda\right) u_\nu v_\nu - \left(u_\nu^2 - v_\nu^2\right) \Re\left\{\Delta\right\} = 0 \tag{D18a}$$

$$- \left(u_\nu^2 + v_\nu^2\right) \Im\left\{\Delta\right\} = 0. \tag{D18b}$$

Using the unitarity condition of Eq. (D12), Eq. (D18b) implies that Δ is a real number. By substitution, we can show that Eq. (D18a) is satisfied by

$$\begin{aligned} u_\nu^2 &= \frac{1}{2}\left(1 + \frac{\epsilon_\nu - \lambda}{\sqrt{\left(\epsilon_\nu - \lambda\right)^2 + \Delta^2}}\right) \\ v_\nu^2 &= \frac{1}{2}\left(1 - \frac{\epsilon_\nu - \lambda}{\sqrt{\left(\epsilon_\nu - \lambda\right)^2 + \Delta^2}}\right), \end{aligned} \tag{D19}$$

and the signs of u_ν and v_ν must be such that

$$u_\nu v_\nu = \sqrt{u_\nu^2 v_\nu^2} = \frac{\Delta}{2\sqrt{\left(\epsilon_\nu - \lambda\right)^2 + \Delta^2}} \tag{D20}$$

If we could determine the parameters Δ and λ, we could deduce the u_ν and v_ν coefficients using Eq. (D19) and the Hamiltonian in Eq. (D16) as well. In principle, we can calculate Δ from its definition in Eq. (D6)

$$\begin{aligned} \Delta &= G\sum_{\nu>0} \langle a_{\overline{\nu}} a_\nu \rangle \\ &= G\sum_{\nu>0} \left(u_\nu^2 \langle b_{\overline{\nu}} b_\nu \rangle - v_\nu^2 \langle b_\nu^\dagger b_{\overline{\nu}}^\dagger \rangle\right) + G\sum_{\nu>0} u_\nu v_\nu (1 - \underbrace{\langle b_\nu^\dagger b_\nu \rangle}_{n_\nu} - \underbrace{\langle b_{\overline{\nu}}^\dagger b_{\overline{\nu}} \rangle}_{n_{\overline{\nu}}}), \end{aligned} \tag{D21}$$

where we've defined the quasi-particle numbers n_ν and $n_{\overline{\nu}}$ (these are numbers, not operators). Note that the quasi-particle numbers must be real because

$$n_\nu^* = \langle b_\nu^\dagger b_\nu \rangle^* = \langle (b_\nu)^\dagger (b_\nu^\dagger)^\dagger \rangle = \langle b_\nu^\dagger b_\nu \rangle = n_\nu \tag{D22}$$

and similarly for $n_{\overline{\nu}}$. Thus far, we have not specified the nature of the wave functions used to calculate the mean values like $\langle b_{\overline{\nu}} b_\nu \rangle$ and $\langle b_\nu^\dagger b_{\overline{\nu}}^\dagger \rangle$. If we choose wave functions ($|\psi\rangle$) that are constructed from a quasi-particle vacuum ($|\tilde{0}\rangle$) using the $b^\dagger$ operators, then we must have

$$\begin{aligned} \langle b_{\overline{\nu}} b_\nu \rangle &\equiv \langle \psi | b_{\overline{\nu}} b_\nu | \psi \rangle = 0 \\ \langle b_\nu^\dagger b_{\overline{\nu}}^\dagger \rangle &\equiv \langle \psi | b_\nu^\dagger b_{\overline{\nu}}^\dagger | \psi \rangle = 0 \end{aligned} \tag{D23}$$

because the b operators acting on the bra and the ket produce orthogonal wave functions. The expression for Δ in Eq. (D21) reduces to

$$\Delta = G\sum_{\nu>0} u_\nu v_\nu (1 - n_\nu - n_{\overline{\nu}}). \tag{D24}$$

Inserting Eq. (D20) into Eq. (D24), we get the general form of the well-known gap equation [39]

$$\sum_{\nu>0} \frac{1 - n_\nu - n_{\overline{\nu}}}{\sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}} = \frac{2}{G} \tag{D25}$$

Another useful equation can be obtained by requiring that the number operator, defined in Eq. (D9), reproduce the known number of particles $\mathcal{N}$, on average,

$$\begin{aligned}
&\langle \hat{\mathcal{N}} \rangle = \mathcal{N} \\
\Rightarrow\ & \left\langle \sum_{\nu>0} (u_\nu^2 - v_\nu^2)\left(b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}}\right) + 2\sum_{\nu>0} v_\nu^2 + 2\sum_{\nu>0} u_\nu v_\nu \left(b_\nu^\dagger b_{\overline{\nu}}^\dagger + b_{\overline{\nu}} b_\nu\right) \right\rangle = \mathcal{N} \\
\Rightarrow\ & \sum_{\nu>0} (u_\nu^2 - v_\nu^2)(n_\nu + n_{\overline{\nu}}) + 2\sum_{\nu>0} v_\nu^2 = \mathcal{N} \\
\Rightarrow\ & \sum_{\nu>0} \frac{\epsilon_\nu - \lambda}{\sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}} (n_\nu + n_{\overline{\nu}}) + \sum_{\nu>0} \left(1 - \frac{\epsilon_\nu - \lambda}{\sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}} \right) = \mathcal{N}
\end{aligned} \tag{D26}$$

where we've used Eq. (D23) to cancel the mean values of off-diagonal terms. In typical applications, the averages in Eqs. (D25) and (D26) are taken with respect to the quasi-particle vacuum. In that case, there are no quasi-particles in the states ν and $n_\nu = n_{\overline{\nu}} = 0$. Eqs. (D25) and (D26) then reduce to more familiar forms (see, e.g., [42]), which can be solved for the values of Δ and λ given the interaction strength G, the number of particles $\mathcal{N}$, and a set of single-particle energies ϵ_ν.

We return to the Hamiltonian in Eq. (D16) and simplify it using Eqs. (D19), (D20), and (D25) along with the conditions $\Delta = \Delta^*$ and $w_\nu = w_\nu^* = 0$,

$$\begin{aligned}
H &= \underbrace{\sum_{\nu>0} \left(\epsilon_\nu - \lambda - \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2} \right) + \frac{\Delta^2}{G}}_{E_0} \\
&\quad + \sum_{\nu>0} \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2} \left(b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}} \right),
\end{aligned} \tag{D27}$$

where we've identified the ground-state energy $E_0 \equiv \langle \tilde{0} | H | \tilde{0} \rangle$ (remember that, by definition, $\langle \tilde{0} | b_\nu^\dagger b_\nu | \tilde{0} \rangle = \langle \tilde{0} | b_{\overline{\nu}}^\dagger b_{\overline{\nu}} | \tilde{0} \rangle = 0$).

The grand partition function, which we defined in Eqs. (19) and (28) can be written for a Hamiltonian operator as a trace,

$$\begin{aligned}
Z &\equiv Tr\, e^{-\beta H} \\
&= \sum_i \langle \Psi_i | e^{-\beta H} | \Psi_i \rangle,
\end{aligned} \tag{D28}$$

where we've written out the trace explicitly in terms of a sum over all possible particle numbers and configurations represented by the wave functions $|\Psi_i\rangle$. Note that the Hamiltonian H already contains the Lagrange multiplier for the particle number thanks to Eq. (D9), so that Eq. (D28) does represent the grand partition function, and not just the partition function. The Lagrange multiplier λ is in fact the Fermi energy ϵ_F we've used throughout this manuscript, with the usual notation adapted from Eq. (46)

$$\lambda \equiv \frac{\alpha}{\beta} = \epsilon_F. \tag{D29}$$

The wave functions $|\Psi_i\rangle$ are eigenstates of the Hamiltonian H, therefore we can write

$$\begin{aligned} Z(\alpha,\beta) &= \sum_i \left\langle \Psi_i \middle| e^{-\beta H} \middle| \Psi_i \right\rangle \\ &= \sum_i e^{-\beta \langle \Psi_i | H | \Psi_i \rangle}, \end{aligned} \tag{D30}$$

which is reminiscent of Eq. (28). The Hamiltonian in question is given by Eq. (D27). The ground-state energy E_0 defined in Eq. (D27) is independent of the configuration (i.e., it does not depend on the distribution of quasi particles among the states, and therefore it does not depend on the index i in Eq. (D30) number of quasi-particles in the system), thus

$$\begin{aligned} Z(\alpha,\beta) &= e^{-\beta E_0} \sum_i e^{-\beta \left\langle \Psi_i \middle| \sum_{\nu>0} \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2} \left(b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}} \right) \middle| \Psi_i \right\rangle} \\ &= e^{-\beta E_0} \sum_i e^{-\beta \sum_{\nu>0} \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2} \left(n_\nu^{(i)} + n_{\overline{\nu}}^{(i)} \right)}, \end{aligned} \tag{D31}$$

where the superscripts "(i)" on the quasi-particle numbers $n_\nu^{(i)}$ and $n_{\overline{\nu}}^{(i)}$ serve as a reminder that each configuration i may contain different numbers of quasi-particles in each state ν or $\overline{\nu}$. We've already seen how sums over configurations such as the one in Eq. (D31) can be simplified in section II B 2, the answer is given by Eq. (32). Thus we write

$$\ln Z(\alpha,\beta) = -\beta E_0 + 2 \sum_{\nu>0} \ln \left(1 + e^{-\beta \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}} \right), \tag{D32}$$

where the factor of 2 in front of the sum comes from the fact that the configuration sums over ν and $\overline{\nu}$ are equal. For convenience of notation, we define the quasi-particle energy

$$E_\nu \equiv \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}. \tag{D33}$$

The gap equation, Eq. (D25), which is valid at zero temperature, must be generalized to finite temperatures. In order to do this, we replace the average with respect to a single wave function used in Eq. (D25) by the thermal average of an operator $\mathcal{O}$, defined as

$$\langle \mathcal{O} \rangle_{th} \equiv \frac{Tr\, \mathcal{O} e^{-\beta H}}{Tr\, e^{-\beta H}} = \frac{1}{Z} Tr\, \mathcal{O} e^{-\beta H}. \tag{D34}$$

In the case of the average of $b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}}$, we can use a mathematical trick to evaluate the thermal average

$$\begin{aligned} \langle b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}} \rangle_{th} &= \frac{1}{Z} Tr \left\{ \left(b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}} \right) e^{-\beta E_0 - \beta \sum_{\mu>0} E_\mu \left(b_\mu^\dagger b_\mu + b_{\overline{\mu}}^\dagger b_{\overline{\mu}} \right)} \right\} \\ &= \frac{1}{Z} Tr \left\{ -\frac{e^{-\beta E_0}}{\beta} \frac{\partial}{\partial E_\nu} e^{-\beta \sum_{\mu>0} E_\mu \left(b_\mu^\dagger b_\mu + b_{\overline{\mu}}^\dagger b_{\overline{\mu}} \right)} \right\} \\ &= -\frac{1}{\beta} e^{-\beta E_0} \frac{\frac{\partial}{\partial E_\nu} Tr \left[e^{\beta E_0} e^{-\beta H} \right]}{Tr e^{-\beta H}} \\ &= -\frac{1}{\beta} \frac{\partial}{\partial E_\nu} \ln \left(e^{\beta E_0} Z \right) \\ &= \frac{2 e^{-\beta E_\nu}}{1 + e^{-\beta E_\nu}}, \end{aligned} \tag{D35}$$

where we've used Eq. (D32) to derive the last line. We've also kept in mind the fact that E_0 contains a dependence on the quasi-particle energies E_ν, which we do not want to include inside the differentiation in Eq. (D35). Then Eq. (D25) becomes

$$\sum_{\nu>0} \frac{1-\langle b_\nu^\dagger b_\nu + b_{\overline{\nu}}^\dagger b_{\overline{\nu}}\rangle_{th}}{E_\nu} = \frac{2}{G}$$
$$\Rightarrow \sum_{\nu>0} \frac{1}{E_\nu} \tanh\frac{\beta E_\nu}{2} = \frac{2}{G}. \tag{D36}$$

In the zero-temperature limit (i.e., $\beta \to \infty$), it can be shown that Eq. (D36) reduces to Eq. (D25) for the quasi-particle vacuum (i.e., with $n_\nu = n_{\overline{\nu}} = 0$).

We can also calculate the energy and particle number using either the thermal-average formula in Eq. (D34), or the more familiar saddle-point conditions of Eq. (21), which can be derived from Eq. (D34). To calculate Eq. (21), we will need the derivatives of E_ν with respect to the Lagrange multipliers α and β

$$\begin{aligned}\frac{\partial}{\partial\alpha}E_\nu &= \frac{\partial}{\partial\alpha}\sqrt{\left(\epsilon_\nu - \frac{\alpha}{\beta}\right)^2 + \Delta^2} = -\frac{1}{\beta}\times\frac{\epsilon_\nu-\lambda}{E_\nu}\\ \frac{\partial}{\partial\beta}E_\nu &= \frac{\partial}{\partial\beta}\sqrt{\left(\epsilon_\nu - \frac{\alpha}{\beta}\right)^2 + \Delta^2} = \frac{\lambda}{\beta}\times\frac{\epsilon_\nu-\lambda}{E_\nu},\end{aligned} \tag{D37}$$

then Eq. (21b), applied to Eq. (D32), gives the number of particles $\mathcal{N}$

$$\mathcal{N} = \frac{\partial}{\partial\alpha}\ln Z = \sum_{\nu>0}\left[1 - \frac{\epsilon_\nu-\lambda}{E_\nu}\tanh\frac{\beta E_\nu}{2}\right]. \tag{D38}$$

Similarly, we calculate the energy, using Eqs. (21a), (D32), the gap equation (D36), and the definition of E_0 in Eq. (D27)

$$\begin{aligned}E = -\frac{\partial}{\partial\beta}\ln Z &= E_0 + \beta\frac{\partial E_0}{\partial\beta} + 2\sum_{\nu>0}\frac{e^{-\beta E_\nu}}{1+e^{-\beta E_\nu}}\left(E_\nu + \beta\frac{\partial E_\nu}{\partial\beta}\right)\\ &= \sum_{\nu>0}\epsilon_\nu\left[1 - \frac{\epsilon_\nu-\lambda}{E_\nu}\tanh\frac{\beta E_\nu}{2}\right] - \frac{\Delta^2}{G}.\end{aligned} \tag{D39}$$

The procedure used to construct a state density from the grand partition function has already been discussed in section II B 1. The state density is given explicitly in Eq. (22). The necessary partial derivatives are given in [39]. The results above can also be readily generalized to the case of both protons and neutrons. The state density in Eq. (22) generalizes to

$$w(A,E) \approx \frac{e^S}{2\pi\sqrt{D}}, \tag{D40}$$

where S is the entropy defined as

$$S = \ln Z(\alpha,\beta) - \alpha A + \beta E \tag{D41}$$

We can further generalize the results to the case where both protons and neutrons are treated in the BCS formalism. The results of Eqs. (D32), (D38), and (D39) can be applied separately to protons and neutrons, in that case we ultimately obtain separate entropies for the systems of Z protons and N neutrons

$$\begin{aligned}S_p &\equiv \ln Z_p(\alpha_p,\beta_p) - \alpha_p Z + \beta E_p\\ S_n &\equiv \ln Z_n(\alpha_n,\beta_n) - \alpha_n N + \beta E_n,\end{aligned} \tag{D42}$$

with

$$\begin{aligned} A &= Z + N \\ E &= E_p + E_n. \end{aligned} \tag{D43}$$

The state density is a generalization of Eq. (D40), formally given by Eq. (25). We have

$$w(Z, N, E) \approx \frac{e^{S_p + S_n}}{(2\pi)^{3/2}\sqrt{D}}. \tag{D44}$$

There are three Lagrange multipliers in Eq. (D44), determined by Eqs. (D38) and (D39), and the D matrix is a 3×3 matrix.

APPENDIX E: THE STRUTINSKY SHELL CORRECTION

In section IV we separated the energy of the system into a smooth and oscillating part explicitly for a toy shell model, and qualitatively for more general cases. However, the derivation based on the grand partition function is not well suited for a quantitative evaluation in the case of a general set of single-particle states ϵ_n. The Strutinsky shell-correction method is more commonly used to effect the separation. We will present this technique, closely following the development in [32]. We return to the general single-particle spectrum

$$g(\epsilon) = \sum_{n=1}^{\infty} \delta(\epsilon - \epsilon_n). \tag{E1}$$

We will divide $g(\epsilon)$ into a smooth part $\tilde{g}(\epsilon)$ and a part representing local fluctuations, $\delta g(\epsilon)$:

$$g(\epsilon) = \tilde{g}(\epsilon) + \delta g(\epsilon), \tag{E2}$$

and calculate an energy contribution $\tilde{\epsilon}(n)$ that varies smoothly with the particle number n. The shell correction for a system of N particles will then be given by

$$\Delta E_{sc} = \sum_{n=1}^{N} \epsilon_n - \int_0^N \tilde{\epsilon}(n) dn \tag{E3}$$

We start by expanding the δ functions in Eq. (E1) using Hermite polynomials [44], weighted by a Gaussian function

$$\delta(x) = e^{-x^2} \sum_{m=0}^{\infty} c_m H_m(x). \tag{E4}$$

The Gaussian function is needed to reproduce the localization imposed by the delta function. The expansion coefficients c_m can be determined using the orthogonality properties of the Hermite polynomials, [44]

$$\int_{-\infty}^{\infty} H_k(x) H_m(x) e^{-x^2} dx = 2^m m! \sqrt{\pi}\, \delta_{k,m}. \tag{E5}$$

Then we have

$$\begin{aligned} \int_{-\infty}^{\infty} H_k(x)\delta(x) dx &= \sum_{m=0}^{\infty} c_m \int_{-\infty}^{\infty} H_k(x) H_m(x) e^{-x^2} dx \\ \Rightarrow\ c_k &= \frac{H_k(0)}{2^k k! \sqrt{\pi}}. \end{aligned} \tag{E6}$$

The $H_k(0)$ are Hermite numbers with well-known values [44]. The expansion coefficients are

$$c_k = \begin{cases} \frac{(-1)^{k/2}}{\sqrt{\pi}2^k(k/2)!} & k \text{ even} \\ 0 & k \text{ odd} \end{cases} \tag{E7}$$

We also introduce a scaling parameter $\gamma > 0$ to control the range of the Gaussian weight factor in Eq. (E4). Thus we replace the delta functions in Eq. (E1) with

$$\delta(x) \rightarrow \frac{1}{\gamma}\delta\left(\frac{x}{\gamma}\right). \tag{E8}$$

Note that the substitution in Eq. (E8) does not affect the count of levels in Eq. (E1) because

$$\int_{-\infty}^{\infty} dx \frac{1}{\gamma}\delta\left(\frac{x}{\gamma}\right) = \int_{-\infty}^{\infty} d\left(\frac{x}{\gamma}\right)\delta\left(\frac{x}{\gamma}\right) = \int_{-\infty}^{\infty} \delta(x) = 1 \tag{E9}$$

We can therefore expand $g(\epsilon)$ in Eq. (E1) in terms of Hermite polynomials

$$g(\epsilon) = \frac{1}{\gamma}\sum_{n=1}^{\infty} e^{-u_n^2} \sum_{m=0}^{\infty} c_m H_m(u_n), \tag{E10}$$

where we've defined

$$u_n \equiv \frac{\epsilon - \epsilon_n}{\gamma}. \tag{E11}$$

The Hermite polynomials become increasingly oscillatory as their order increases, so we keep only the first p terms to reproduce the smooth contribution in $g(\epsilon)$ (where p is small). The remaining terms in the expansion can be identified with the oscillatory contribution.

The number of particles $\tilde{n}(\epsilon)$ up to energy ϵ, which varies as a smooth function of the energy can be calculated from the smooth portion of $g(\epsilon)$, obtained from the first p terms in Eq. (E10)

$$\begin{aligned} \tilde{n}(\epsilon) &= \int_{-\infty}^{\epsilon} \tilde{g}(\epsilon')d\epsilon' \\ &= \sum_{n=1}^{\infty}\sum_{m=0}^{p} c_m \underbrace{\frac{1}{\gamma}\int_{-\infty}^{\epsilon} d\epsilon' e^{-(u_n')^2} H_m(u_n')}_{I_m(u_n)}, \end{aligned} \tag{E12}$$

where $u_n' \equiv (\epsilon' - \epsilon_n)/\gamma$, and where we've defined the integral $I_m(u_n)$. To calculate this integral, we use the alternate form of the Hermite polynomials [44]

$$H_m(x) = \frac{1}{2}(-1)^m\sqrt{\pi}e^{x^2}\frac{d^{m+1}}{dx^{m+1}}\mathit{erf}(x), \tag{E13}$$

where $\mathit{erf}(x)$ is the error function. Then we can show that

$$\begin{aligned} I_m(u_n) &\equiv \frac{1}{\gamma}\int_{-\infty}^{\epsilon} d\epsilon' e^{-(u_n')^2} H_m(u_n') \\ &= \int_{-\infty}^{u_n} dx\, e^{-x^2} H_m(x) \\ &= \int_{-\infty}^{u_n} dx \frac{1}{2}(-1)^m\sqrt{\pi}\frac{d^{m+1}}{dx^{m+1}}\mathit{erf}(x) \\ &= -e^{-u_n^2} H_{m-1}(u_n), \end{aligned} \tag{E14}$$

where the last line is valid for $m \geq 1$. In the special case $m = 0$, we express the result directly in terms of the error function. The integral in the last step of Eq. (E14) gives

$$I_0(u_n) = \frac{\sqrt{\pi}}{2}\left[1 + \mathit{erf}(u_n)\right]. \tag{E15}$$

Using the explicit values of the integrals in Eqs. (E14) and (E15), we expand the expression for $\tilde{n}(\epsilon)$ in Eq. (E12)

$$\tilde{n}(\epsilon) = \sum_{n=1}^{\infty}\left\{\frac{1}{2}\left[1 + \mathit{erf}(u_n)\right] - e^{-u_n^2}\sum_{m=1}^{p} c_m H_{m-1}(u_n)\right\}. \tag{E16}$$

In particular, for a system of N particles, we can determine the Fermi energy λ by solving numerically the equation

$$\tilde{n}(\lambda) = N, \tag{E17}$$

where $\tilde{n}(\lambda)$ is calculated using Eq. (E16).

Finally, we turn to the calculation of that part of the system's energy which varies smoothly with particle number, introduced in Eq. (E3). For N particles, this smooth energy contribution is

$$\tilde{E} \equiv \int_0^N dn\, \tilde{\epsilon}(n) = \int_{-\infty}^{\lambda} d\tilde{\epsilon}\,\frac{dn}{d\tilde{\epsilon}}\tilde{\epsilon}(n) = \int_{-\infty}^{\lambda} d\tilde{\epsilon}\,\tilde{g}(\tilde{\epsilon})\tilde{\epsilon} = \int_{-\infty}^{\lambda} d\epsilon\,\tilde{g}(\epsilon)\epsilon, \tag{E18}$$

where in the last equality, we've treated $\tilde{\epsilon}$ as a dummy variable. Taking the first $m \leq p$ terms in the Hermite polynomial expansion in Eq. (E10) we calculate

$$\tilde{E} = \int_{-\infty}^{\lambda} d\epsilon\,\tilde{g}(\epsilon)\epsilon = \sum_{n=1}^{\infty}\sum_{m=0}^{p} c_m \underbrace{\frac{1}{\gamma}\int_{-\infty}^{\lambda} d\epsilon\,\epsilon\, e^{-u_n^2} H_m(u_n)}_{I'_m(\overline{u}_n)}, \tag{E19}$$

where $\overline{u}_n \equiv (\lambda - \epsilon_n)/\gamma$. The integral $I'_m(\overline{u}_n)$ can be further simplified

$$\begin{aligned} I'_m(\overline{u}_n) &= \frac{1}{\gamma}\int_{-\infty}^{\overline{u}_n} \gamma dx\,(\epsilon_n + \gamma x)e^{-x^2}H_m(x) \\ &= \epsilon_n \underbrace{\int_{-\infty}^{\overline{u}_n} dx\, e^{-x^2}H_m(x)}_{I_m(\overline{u}_n)} + \gamma \underbrace{\int_{-\infty}^{\overline{u}_n} dx\, x\, e^{-x^2}H_m(x)}_{I''_m(\overline{u}_n)}, \end{aligned} \tag{E20}$$

where we've renamed the dummy integration variable as $x \equiv u_n$, and the integral I_m was calculated in Eqs. (E14) and (E15). The new integral, $I''_m(\overline{u}_n)$, can be evaluated using the recurrence relation [44]

$$\frac{d}{dx}H_m(x) = 2mH_{m-1}(x), \tag{E21}$$

then, by parts,

$$\begin{aligned} I''_m(\overline{u}_n) &= -\frac{1}{2}\, e^{-x^2}H_m(x)\Big|_{x\to-\infty}^{x=\overline{u}_n} + \frac{1}{2}\int_{-\infty}^{\overline{u}_n} dx\, e^{-x^2}\frac{d}{dx}H_m(x) \\ &= -\frac{1}{2}e^{-\overline{u}_n^2}H_m(\overline{u}_n) + m\int_{-\infty}^{\overline{u}_n} dx\, e^{-x^2}H_{m-1}(x) \\ &= -\frac{1}{2}e^{-\overline{u}_n^2}H_m(\overline{u}_n) + mI_{m-1}(\overline{u}_n). \end{aligned} \tag{E22}$$

Combining Eqs. (E20) and (E22), and using Eq. (E14) we get, for $m \geq 2$

$$I'_m(\overline{u}_n) = -e^{-\overline{u}_n^2}\left[\frac{\gamma}{2}H_m(\overline{u}_n) + \epsilon_n H_{m-1}(\overline{u}_n) + m\gamma H_{m-2}(\overline{u}_n)\right] \tag{E23}$$

For the special case $m = 0$, we have

$$I''_0(\overline{u}_n) = \int_{-\infty}^{\overline{u}_n} dx\, x\, e^{-x^2} = -\frac{1}{2}e^{-\overline{u}_n^2}, \tag{E24}$$

and therefore,

$$\begin{aligned} I'_0(\overline{u}_n) &= \epsilon_n I_0(\overline{u}_n) + \gamma I''_0(\overline{u}_n) \\ &= \frac{\sqrt{\pi}}{2}\epsilon_n\left[1 + erf(\overline{u}_n)\right] - \frac{\gamma}{2}e^{-\overline{u}_n^2}. \end{aligned} \tag{E25}$$

We do not need to calculate the special case $m = 1$ because, according to Eq. (E7), $c_1 = 0$ and the $m = 1$ term vanishes.

Returning to Eq. (E19), and using Eqs. (E20) and (E25), we write

$$\begin{aligned} \tilde{E} &= \sum_{n=1}^{\infty}\left\{\frac{1}{2}\epsilon_n\left[1 + erf(\overline{u}_n)\right] - \frac{\gamma}{2\sqrt{\pi}}e^{-\overline{u}_n^2}\right. \\ &\quad \left. -e^{-\overline{u}_n^2}\sum_{m=1}^{p} c_m\left[\frac{\gamma}{2}H_m(\overline{u}_n) + \epsilon_n H_{m-1}(\overline{u}_n) + m\gamma H_{m-2}(\overline{u}_n)\right]\right\}. \end{aligned} \tag{E26}$$

Recalling Eq. (E3), the shell correction energy can then be calculated for any set of single-particle states ϵ_n using Eq. (E26)

$$\Delta E_{sc} = \sum_{n=1}^{N}\epsilon_n - \tilde{E} \tag{E27}$$

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[45] For $a > 0$, $Prob(x \leq x_0) = \int_{-\infty}^{x_0} dx'\, f(x') \Rightarrow Prob(ax \leq x_0) = \int_{-\infty}^{x_0/a} dx'\, f(x') = \int_{-\infty}^{x_0} \frac{dx''}{a}\, f(\frac{x''}{a})$. Thus if x has probability distribution $f_G(x;0,1)$, then $M \equiv \sqrt{n}\sigma_i x$ has distribution $\frac{1}{\sqrt{n}\sigma_i} f(\frac{x}{\sqrt{n}\sigma_i};0,1)$.

[46] In the most general form of the Laplace inversion integral, also known as a Bromwich integral, the integration limits run from $\gamma - i\infty$ to $\gamma + i\infty$, where γ is real and chosen to exclude any singularities in the integrand. For simplicity, we assume we can choose $\gamma = 0$.

[47] In fact, we should label the n_ν by the index i to indicate that each many-body state i corresponds to a particular arrangement of particles among the single-particle states, but we will refrain from doing this to keep the notation as simple as possible.

[48] n-fold rotations refer to rotations through an angle $2\pi/n$.

[49] Strictly speaking, an operator and its matrix representation are not the same thing, and the matrix element of an operation R is often denoted by a different symbol, for example $D(R)$.

[50] This is similar to the general form of Eq. (102), but we've neglected the intrinsic spin and assumed $\hat{J}_i = \hat{R}_i$.

[51] This is the reason why the saddle-point approximation is sometimes called the "stationary-phase approximation".

[52] This is the origin of the term "saddle-point approximation".